QUADRATIC APPROXIMATION AND ITS APPLICATION TO ACCELERATION OF CONVERGENCE

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CHAPTER PAGE

ABSTRACT

This thesis is a study of quadratic approximation and its application to the acceleration of slowly converging sequences arising, in particular, from the numerical integration of an (improper) integral with singularity.

It commences by considering the convergence of the quadrature approximants to the integral with singularity. The location of singularity affects the rate of convergence when the process of ignoring the singularity is used. Numerical results show that most of the quadratures can cater for the integral with a singularity located at the end points of the interval (or subintervals) of integration.

Then the rate of convergence is considered. A number of accelerators such as the Romberg method, Aitken Δ^2 process and the ε-algorithm are compared. The ε-algorithm is not as good as the modified Romberg method, but better than the unmodified Romberg and Aitken Δ^2 process.

Since the ε-algorithm is based on the use of the Pade approximation, a general algorithm for the calculation of rational approximations is developed.

The quadratic approximation, which is an extension of Pade approximation, is then studied. The general forms of expressing this approximation by the polynomial coefficients are given. A recursive algorithm for the construction of the approximation is derived. This algorithm is based on the MNA (Muhlbach-Neville-

Aitken) algorithm which can be applied to the rational interpolation and Pade approximation. This approximation can be applied to speed up the convergence of a converging sequence and can be extended to the interpolation. With the general recursive algorithm, all possible quadratic approximants and interpolants can be constructed.

The use of the quadratic approximation for linearly convergent sequences, monotonic and alternating series is illustrated. Numerical results show that the convergence of a suitable quadratic approximant is faster than Pade approximant if convergence of the Pade approximant is not fast. Some properties of quadratic approximations are derived.

CHAPTER 1

INTRODUCTION

This thesis is mainly a study of quadratic approximation and its application to accelerating the convergence of a converging sequence. The quadratic approximation is an extension of Pade approximation. The research is motivated by attempting to find an effective method for evaluating an integral with (integrable) singularity* and an effective acceleration process for the convergence of a sequence of quadrature approximants to the integral with singularity. Such integrals often cannot be readily handled by ordinary numerical quadrature. A number of methods have been developed to deal with an integral with singularity. These methods can be classified by three different approaches:

(i) Transform the integral with singularity to a proper integral (i.e. with no singularity).

(ii) Modify a classical technique for evaluating a proper integral to the case where a singularity occurs.

(iii) Ignore or avoid the singularity. 'Ignore' means whenever the singularity appears, the function value assigned is zero and 'avoid' is using a numerical quadrature which does not involve the singularity.

An investigation of the process of ignoring the singularity is discussed. This process was proposed by Davis and Rabinowitz [2] in 1965. Since then, a number of papers on ignoring the singularity in numerical quadrature have been published. These

* In this thesis singularity will always mean integrable singularity.

include the extension and generalization of this process and the study of the nature of the singularity.

A careful study of the location of the singularity appears to have been overlooked and this is discussed in Chapter 2. It is found to affect the convergence of numerical integration. Numerical quadratures which include conventional quadrature rules such as the trapezoidal rule, Simpson's rule, Gaussian rule, and others favour the integrand with an endpoint singularity. The convergence to the exact value of the well behaved integrand with endpoint singularity is monotonic. Some quadratures may give slow convergence. However, the rate of convergence can be accelerated by extrapolation processes. A discussion and comparison of various extrapolation techniques, for example, the Romberg method, Aitken Δ^2 process and the ε-algorithm are given in Chapter three.

It is known that the modified Romberg method, applied to a function with an endpoint singularity, is an efficient procedure but at the cost of knowing the appropriate asymptotic error expansions for the quadrature. The ε-algorithm, which does not require the user to supply these parameters, is not as good as the modified Romberg method, but gives substantially better results than some other extrapolation processes such as the unmodified Romberg's method, Aitken Δ^2 process and rational extrapolation. Much research comparing the extrapolation processes to various functions has been carried out in recent years.

Starting from a study of Pade approximation, an attempt is made to extend the ε-algorithm, which is the application of the well-known Pade approximation. There has been some recent interest in the generalization and extension of Pade approximation. The generalization of the two dimensional Pade approximation to three dimensional quadratic approximation was considered in Pade's original manuscript [4] in 1892, but it was not developed until 1974. Shafer [3] considered this idea and showed the advantages of employing quadratic approximation applied to some particular examples such as $\tan^{-1}x$, $\cos^{-1}x$, $\sin^{-1}x$, $\log(1+x)$ and e^x. Since then, the quadratic approximation has been used in approximating experimental results in physics and chemistry. In contrast, very few studies concerning the structure and the method of derivation of this type of approximation were then known. The present work has resulted from attempts to study these problems.

In this study, the structure, derivation and application of the quadratic approximation have been investigated. Since it is a higher dimensional extension of Pade approximation, it has similar basic structure and common properties, but the increase in dimension leads to a more complicated computation. It is found that the generalized MNA (Muhlbach-Neville-Aitken) algorithm by Brezinski [1] can be extended to the computation of quadratic approximations. This algorithm not only can be applied to the general interpolation problem, orthogonal polynomial and Pade-type approximants but also can be used for rational interpolation and generalized to Pade approximation.

Chapter four extends this algorithm to rational interpolation and Chapter five extends this algorithm to Pade approximation. These form the basis of a further extension to quadratic approximation

With this preparation, Chapter six concentrates on developing the quadratic approximation. This includes the general form of polynomial coefficients of the quadratic approximation to a function f(x) which can be expressed as a formal power series. The algorithm for constructing this approximation is derived and the approximation is applied to the acceleration of the convergence of sequences. It is essentially a generalization of the ε-algorithm based on the Pade approximation. Moreover, the idea of interpolation by quadratic approximation is also introduced and the same general algorithm can be used to calculate an interpolatory quadratic approximation.

In Chapter seven some properties of this approximation are studied and the application of this approximation to various convergent sequences has been tested.

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CHAPTER 2

LOCATION OF THE SINGULARITY IN NUMERICAL QUADRATURE

2.1 INTRODUCTION

A number of methods have been found for the numerical integration of functions with integrable singularities. These include proceeding to the limit, changes of variable, elimination of the singularity by subtraction, use of integration formulas which absorb the singularity into a fixed weighting function (e.g. Gauss type), avoiding or ignoring the singularity. For further references see [2].

Davis and Rabinowitz [1] investigated the process of ignoring the singularity in numerical quadrature. They show that if the singularity occurs at a rational point and if the integrand is monotonic in a neighborhood of the singularity, then ignoring the singularity is a theoretically valid process for a large class of sequences of composite rules. Rabinowitz [12] extended the class of composite rules to include those based on quadrature formulas with algebraic nodes. Miller [8] replaced the assumption that the integrand is monotonic in a neighborhood of the singularity by a more general condition that the integrand can be dominated by a monotonic, integrable function. A few years later, Rabinowitz [13] generalized the results so that the weights in the quadrature formulas are not required to be positive nor the abscissas to be rational or algebraic.

In this chapter, a technique for locating the singularity, whether it is rational or irrational, at an end point of the interval of integration in the numerical quadrature is given. It is shown that the convergence to the exact value of the integral is then monotonic, though the convergence may be slow. Hence the assumption that the singularity is rational can be dispensed.

In the next section, a brief description of the results given previously in [1],[8] and [12], and the necessary condition of Theorem 2 in [1] are given. This condition leads to a way of allocating the singularity which is discussed in section 2.3. In section 2.4 it can be shown that the integrand with singularity will converge monotonically if one takes care of the location even if it is irrational. Some of the results of the examples in [1] are modified by using this technique in section 2.5.

2.2 THEOREMS OF CONVERGENCE

The theorems about the numerical quadrature of monotonic increasing functions with a singularity in the interval of integration whose integral converges have been found in [1],[12] and [13].

Let f(x) be a nonnegative and monotonic increasing function in the interval $[0,\xi)\xi \leqslant 1$ with a singularity at ξ, with f(x) = 0 in the interval $(\xi,1]$, and such that

$$If = \int_0^1 f(x)dx \text{ is finite.}$$

Let $Q(f) = \sum_{i=1}^{m} \omega_i f(x_i)$ be a simple integration rule such that

$$\omega_i > 0, \quad \sum_{i=1}^{m} \omega_i = 1, \quad 0 \leqslant x_1 < x_2 < \ldots < x_m \leqslant 1 .$$

A composite rule $Q_n(f)$ of mn points which is based on applying Q(f) to each of the n subinterval $[0,\frac{1}{n}]$, $[\frac{1}{n},\frac{2}{n}]$ ... $[\frac{n-1}{n}, 1]$ is the following

$$Q_n(f) = \sum_{i=0}^{n-1} \sum_{k=1}^{m} \omega_k \, f\left(\frac{i}{n} + \frac{x_k}{n}\right) \tag{2.2.1}$$

For each integer $n \geq 1$, define $\xi(n)$ as the abscissa among the mn abscissas of $Q_n(f)$ which is closest to ξ from the left so that $\xi(n) < \xi$. With these definitions, the following results have been shown in [1].

(a) (Theorem 2 in [1]) $Q_n(f)$ converges to If if and only if

$$\lim_{n\to\infty} \frac{1}{n} f(\xi(n)) = 0 \, . \tag{2.2.2}$$

(b) (Theorem 3 in [1]) If $\xi = 1$, then $Q_n(f)$ converges to If .

(c) (Theorem 4 in [1]) If ξ is a rational number $(P/q) < 1$ and the abscissas x_i are rational numbers, then $Q_n(f)$ converges to If.

(d) (Theorem 5 in [1]) Let $0 < \xi < 1$ and suppose that ξ is irrational. If $\frac{1}{2} \leqslant \alpha < 1$ and $f(x)$ is defined by

$$f(x) = \begin{cases} (\xi - x)^{-\alpha} & \text{for } 0 \leqslant x < \xi \\ 0 & \text{for } \xi \leqslant x \leqslant 1 \end{cases} \, .$$

Then $Q_n(f)$ does not converge to If.

(e) (Theorem 6 in [1]) If ξ is an irrational algebraic number and let $0 < \alpha < \frac{1}{2}$ where $f(x)$ is defined as in (d). Then $Q_n(f)$ converges to If. These results have been extended [12] in two ways, i.e.,

(f) (c) has been shown to hold for any Q in which the abscissa x_i are algebraic numbers.

(g) If $\xi = 1$, the quadrature rule Q been extended to a Gaussian quadrature rule of interpolatory type.

In fact, it has also been extended to include the quadrature formulas of maximum algebraic degree with the abscissas x_i being the zeros of the Chebyshev polynomial of the first and second kind in [6].

Instead of assuming f(x) monotonic near $x = \xi$, Miller[8] gives a more general condition for f(x). (Note that Miller's formulation is retained in order to compare the results directly. Thus the non zero part of the function is taken on the right side of the singularity in this case.

Let $f(x) \in M_d(\xi)$

where $M(\xi) = \{f \in C(\xi,1] \cap L_1(\xi,1);\ \ f=0 \text{ on } [0,\xi],\ f \geq 0,\ f \text{ non-increasing on } (\xi,1]\}$

and $M_d(\xi) = \{f \in C(\xi,1] : \exists\ F \in M(\xi) \ni |f(t)| \leq F(t) \text{ on } [0,1]\}$.

Let $Q_n(f) = \sum\limits_{i=1}^{m_n} \omega_{in} f(x_{in}),\quad 0 \leq x_{1n} < x_{2n} <\ldots < x_{m_n,n} \leq 1,$

which includes the previous sequence of composite rules as a special case.

Robinowitz[13] shows that

(h) (Corollary 1 in [13]) If $f \in M_d(\xi)$, $0 \leq \xi \leq 1$ and $|\omega_{in}| \leq k$ $(x_{in} - x_{i-1,n})$ hold, where k and A are positive constants independent of n = 1,2,3 ... and of i = 1(1) m_n such that $x_{in} <$ $A \leq 1$. Then $Q_n(f)$ converges to If if and only if $\lim\limits_{n\to\infty} \omega_{kn}\, f(\xi(n)) = 0$ where $\xi(n)$ is the abscissa x_{kn} in Q_n satisfy $x_{k-1,n} \leq \xi < x_{kn}$.

(i) (Theorem 2 in [13]). If ξ is a rational number $(p/q) < 1$ and $f(x) \in M_d(\xi)$, then $Q_n(f)$ converges to If.

Note that in (h) and (i) the weight ω_{in} need not to be positive and the abscissas x_{in} need not to be rational or algebraic.

(j) (Theorem 3 in [13]). If ξ is irrational, $0 < \xi < 1$ and define $f(x) \in M(\xi)$ by

$$f(x) = \begin{cases} (x-\xi)^{\gamma} |\log^{\beta}(x-\xi)| & \xi < x \leqslant 1 \\ 0 & 0 \leqslant x \leqslant \xi \end{cases}$$

where $-1 \leqslant \gamma \leqslant 0$ and β is arbitrary. The following conclusions hold:

(i) For $-1 < \gamma < -\frac{1}{2}$ and all β and for $\gamma = -\frac{1}{2}$ and $\beta \geqslant 0$, no rule $Q_n(f)$ converges to If.

(ii) For $\gamma = -\frac{1}{2}$ and $0 > \beta \geqslant -\frac{1}{2}$, $Q_n(f)$ does not converge to If.

(iii) For $\gamma = -\frac{1}{2}$ and $\beta < -\frac{1}{2}$ and for $-\frac{1}{2} < \gamma \leqslant 0$ and all β, $Q_n(f)$ converges to If for almost all ξ.

Result (a) is the fundamental theorem for the other results. The necessary and sufficient condition (2.2.2) in (a) is the key of the convergence. In order to satisfy this condition, the singularity needs to be located at an end point of a subinterval. Davis and Rabinowitz [1] concentrate on the nature of the singularity and seem to overlook this point. With this condition the statement of Theorem 2 in [1] is completed. The modification of proof of Theorem 2 in [1] is given below.

Proof. To show if $\lim_{n\to\infty} \frac{1}{n} f(\xi(n)) = 0$, then

$$\lim_{n\to\infty} Q_n(f) = \int_0^1 f(x)\,dx.$$

With the definitions at the beginning, define $k(n)$ as the largest integer such that $k(n)/_n \leqslant \xi(n) < \xi$.

Define $\sigma_i = \sigma_{in}(f) = \sum_{k=1}^{m} \omega_k f(\frac{i}{n} + \frac{x_k}{n})$.

Since $f(x) = 0$ in $\xi \leqslant x \leqslant 1$.

$$\begin{aligned} Q_n(f) &= \frac{1}{n}(\sigma_0 + \dots + \sigma_{n-1}) \\ &= \frac{1}{n}(\sigma_0 + \dots + \sigma_{k(n)-2}) + \frac{1}{n}\sigma_{k(n)-1} + \frac{1}{n}\sigma_{k(n)} \ . \end{aligned}$$

Since $f(x)$ is monotonic in $0 \leqslant x < \xi$ and since $\omega_k > 0$ and $\sum_{k=1}^{m} \omega_k = 1$, $\sigma_0 \leqslant f(\frac{1}{n})$, $\sigma_1 \leqslant f(\frac{2}{n})$ etc. Therefore,

$$\begin{aligned} Q_n(f) &\leqslant \frac{1}{n}(f(\frac{1}{n}) + f(\frac{2}{n}) + \dots + f(\frac{k(n)-1}{n})) + \frac{1}{n} f(\frac{k(n)}{n}) + \frac{1}{n}\sigma_{k(n)} \\ &\leqslant \int_{1/n}^{k(n)/n} f(x)dx + \frac{1}{n} f(\frac{k(n)}{n}) + \frac{1}{n} f(\xi(n)) \\ &\leqslant \int_{1/n}^{k(n)/_n} f(x)dx + \frac{2}{n} f(\xi(n)) \ . \end{aligned}$$

Again, by monotonicity, $\sigma_0 \geqslant f(0)$, $\sigma_1 \geqslant f(\frac{1}{n})$ etc. Furthermore

$$\sigma_{k(n)} = \sum_{j=1}^{m} \omega_i f(\frac{k(n)}{n} + \frac{x_j}{n})$$

Hence if $\omega = \min \{\omega_1, \omega_2 \dots \omega_m\}, \sigma_{k(n)} \geqslant \omega f(\xi(n))$. Therefore

$$\begin{aligned} Q_n(f) &= \frac{1}{n}(\sigma_0 + \sigma_1 + \dots + \sigma_{k(n)-1}) + \frac{1}{n}\sigma_{k(n)} \\ &\geqslant \frac{1}{n}(f(0) + f(\frac{1}{n}) + \dots + f(\frac{k(n)-1}{n})) + \frac{\omega}{n} f(\xi(n)) \\ &\geqslant \int_{0}^{(k(n)-1)/n} f(x)dx + \frac{\omega}{n} f(\xi(n)) \ . \end{aligned}$$

Combining these two inequalities, we obtain

$$\begin{aligned} \frac{\omega}{n} f(\xi(n)) - \int_{(k(n)-1)/n}^{\xi} f(x)dx &\leqslant Q_n(f) - \int_0^1 f(x)dx \\ &\leqslant \frac{2}{n} f(\xi(n)) - \int_0^{1/n} f(x)dx - \int_{k(n)/n}^{\xi} f(x)dx \ . \end{aligned}$$

It follows from the above expression that if $\lim_{n\to\infty} \frac{1}{n} f(\xi(n)) = 0$ then $\lim_{n\to\infty} Q_n(f) = \int_0^1 f(x)dx$.

Conversely, since

$$0 \leqslant \frac{\omega}{n} f(\xi(n)) \leqslant Q_n(f) - \int_0^{(k(n)-1)/n} f(x)dx \tag{2.2.3}$$

If $Q_n(f) \to \int_0^1 f(x)dx = \int_0^{\xi} f(x)dx$, then

$$0 \leqslant \frac{\omega}{n} f(\xi(n)) \leqslant \int_0^{\xi} f(x) - \int_0^{(k(n)-1)/n} f(x)dx$$

$$\leqslant \int_{(k(n)-1)/n}^{\xi(n)} f(x)dx + \int_{\xi(n)}^{\xi} f(x)dx$$

$$\leqslant \left[\xi(n) - \frac{k(n)-1}{n}\right] f(\xi(n)) + 0$$

$$\leqslant \xi(n) f(\xi(n)) - \frac{k(n)}{n} f(\xi(n)) + \frac{1}{n} f(\xi(n)) .$$

Taking the limit on both sides, then

$$0 \leqslant \lim_{n\to\infty} \frac{\omega}{n} f(\xi(n)) \leqslant \lim_{n\to\infty} \frac{1}{n} f(\xi(n))$$

But if ξ lies on an end point of the interval, then

$$\lim_{n\to\infty} \frac{k(n)-1}{n} = \xi$$

and $$\lim_{n\to\infty} \int_0^{(k(n)-1)/n} f(x)dx = \int_0^{\xi} f(x)dx$$

from (2.2.3)

$$0 \leqslant \lim_{n\to\infty} \left\{ \frac{\omega}{n} f(\xi(n))\right\} \leqslant \lim_{n\to\infty} Q_n(f) - \lim_{n\to\infty} \int_0^{(k(n)-1)/n} f(x)dx$$

i.e. $0 \leqslant \omega \lim_{n\to\infty} \frac{1}{n} f(\xi(n)) \leqslant 0$

or $\lim_{n\to\infty} \frac{1}{n} f(\xi(n))$ as required.

2.3 THE LOCATION OF THE SINGULARITY

If the singularity is a rational number P/q, it can be easily located at one of the end points of a subinterval of [a,b] by selecting n as a multiple of q. But if the singularity is irrational, it is not possible to divide the interval to ensure the singularity is at the end point of one of the subintervals. In order to avoid this occurrence the interval can be subdivided from ξ, that is $[a,\xi-\frac{n_1-1}{n}]\ldots[\xi-\frac{1}{n},\xi]$ where n_1 is the largest integer such that $\xi-\frac{n_1}{n}\leqslant a$.

If $0<\xi<1$, then $\int_0^1 f(x)dx = I_1 + I_2$, where I_1 and I_2 are given by

$$I_1=\lim_{x\to\xi^-}\int_0^x f(x)dx \text{ and } I_2=\lim_{x\to\xi^+}\int_x^1 f(x)dx \quad .$$

Then the subintervals will be $[a,\xi-\frac{n_1-1}{n}]\ldots[\xi-\frac{1}{n},\xi],[\xi,\xi+\frac{1}{n}]\ldots$ $[\xi+\frac{n_2-1}{n},b]$ where n_2 is the smallest integer such that $\xi+\frac{n_2}{n}\geqslant b$.

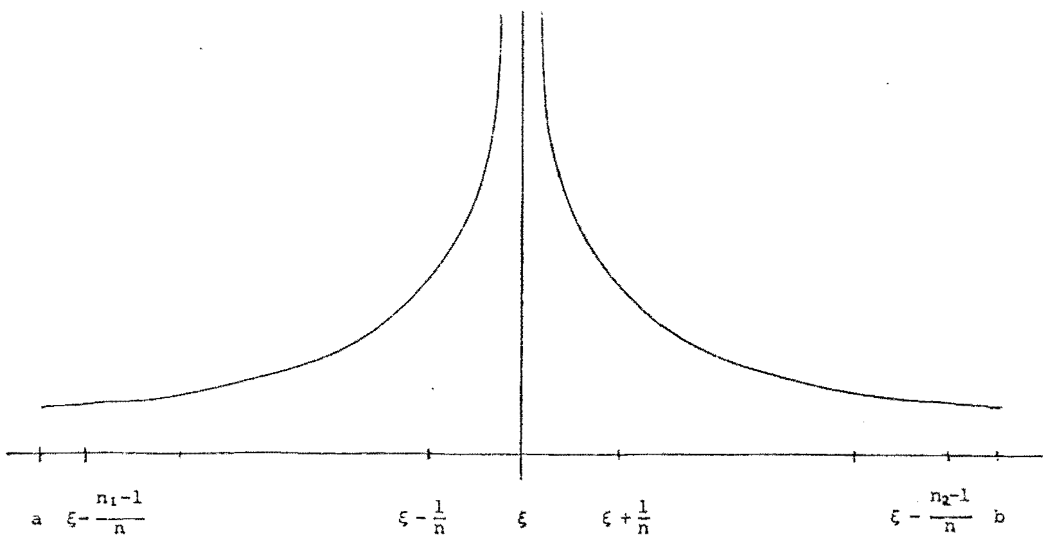

Figure 2.3.1

Note that the first and the last intervals may not be the same as the others, and they have to be treated differently in the composite rule. In this case, k(n) can be generalized from the largest integer to the largest real number in the above proof.

2.4 IRRATIONAL SINGULARITY

For the results (d) and (j) the singularity is irrational. Hence this singularity is allocated to an end point of a sub-interval.

For (d) $f(\xi(n)=[\xi-(\xi-\frac{1}{n})]^{-\alpha} = n^{\alpha}$ for $0 \leq x < \xi$

$$\text{so} \quad \frac{1}{n} f(\xi(n)) = n^{\alpha-1}$$

Since $\frac{1}{2} \leqslant \alpha < 1$ it follows that

$$\lim_{n\to\infty} \frac{1}{n} f(\xi(n)) = 0 \quad \text{and hence}$$

$$Q_n(f) \to If \text{ by (a).}$$

For (j) $\quad \frac{1}{n}f(\xi(n)) =(\frac{1}{n})^{\gamma+1} \; |\log^{\beta}(\frac{1}{n})|$.

For $\gamma > -1$ and $\beta \leq 0$ $\lim_{n\to\infty} \frac{1}{n} f(\xi(n) \to 0$ and hence $Q_n(f) \to If$. However in the case $\beta > 0$ the convergence is very slow and we need to have $n^{\gamma+1} >> |\log^{\beta} (\frac{1}{n})|$ for reasonable computational results.

If $n^{\gamma+1} >> |\log^{\beta} (\frac{1}{n})|$, then taking the logarithm of both sides,

$$(\gamma+1)\log n >> \beta \log(\, |\log(\tfrac{1}{n})| \,)$$

$$\gamma >> \frac{\beta \log|\log (n)|}{\log n} - 1 \text{ for } n > 1.$$

$$\gamma >> \beta \cdot(A-1)$$

where $$A = \frac{\log|\log(n)|}{\log n} \tag{2.4.1}$$

It can be seen that (2.2.2) very much depends on γ,β and n in this case. When $n \to \infty$, $A \to 0$ in (2.4.1) but is very slow, as can be seen in table 2.4.1.

Table 2.4.1

n	A						
1	∞	20	0.0878437	10^3	0.1590404	10^{20}	0.0650515
2	-1.7320208	40	0.1277597	10^4	0.1505150	10^{30}	0.0492374
4	-0.6601042	60	0.1405779	10^6	0.1296919	10^{40}	0.0400515
8	-0.0490194	80	0.1468450	10^8	0.1128862	10^{50}	0.0339794
10	0.0000000	100	0.1505150	10^{10}	0.1000000	10^{100}	0.0200000

As β gets larger a much larger value is needed of n before $\frac{1}{n} f(\xi(n))$ gets small and hence $Q_n(f)$ gets close to If. The examples in the table below show that in this particular case, the convergence is very slow. Note that the expression initially *increases* before beginning a monotonic decrease to zero.

(i) $\gamma = -0.75 \quad \beta = 1$

(ii) $\gamma = -0.75 \quad \beta = 2$

(iii) $\gamma = -0.75 \quad \beta = 3$

(iv) $\gamma = -0.75 \quad \beta = 4$

Table 2.4.2

$\frac{1}{n} f(\xi(n))$ / n	(i)	(ii)	(iii)	(iv)
10	0.56234133	0.56234133	0.56234133	0.56234133
10^2	0.63245554	1.26491108	2.52982216	5.05964432
10^3	0.53348382	1.60045146	4.80135438	14.40406314
10^4	0.40000000	1.60000000	6.40000000	25.60000000
10^5	0.28117067	1.4058533	7.02926663	35.14633312
10^6	0.18973666	1.13841997	6.83051983	40.98311899
10^{10}	0.03162278	0.31622777	3.16227770	31.62277700
10^{15}	0.00266742	0.04001129	0.60016930	9.00253946
10^{20}	0.00020000	0.04000000	0.08000000	1.60000000
10^{30}	0.00000095	0.00002846	0.00085382	0.02561445

2.5 NUMERICAL EXAMPLES

Example 1 (Example 4 in [1])

$$\int_0^1 f(x)dx\ , \quad f(x) = \begin{cases} \dfrac{1}{\sqrt{x-\alpha}} & \text{if } x > \alpha \\ 0 & \text{if } x \leqslant \alpha \end{cases}$$

This integral had been approximated by trapezoidal rule T for

$$\alpha = \frac{1}{16} \pm \frac{1}{512} \quad \text{and} \quad \frac{1}{16} \pm \frac{1}{512} - 5 \times 10^{-8} \text{ in [1].}$$

The results are listed below.

Table 2.5.1

n \ α	$\frac{1}{16}+\frac{1}{512}$	$\frac{1}{16}+\frac{1}{512}-5\times10^{-8}$	$\frac{1}{16}-\frac{1}{512}$	$\frac{1}{16}-\frac{1}{512}-5\times10^{-8}$
1	1.0076	1.0076	1.0042	1.0042
4	1.3861	1.3861	1.3776	1.3776
8	1.7312	1.7312	1.7090	1.7090
16	1.5785	1.5785	2.9764	2.9764
32	1.6905	1.6905	2.3728	2.3728
64	1.7731	1.7731	2.0898	2.0898
128	1.8375	1.8375	1.9596	1.9596
256	1.8966	1.8966	1.9006	1.9006
512	1.8699	29.4910	1.8739	29.4951
1024	1.8888	15.6994	1.8929	15.7034
2048	1.9022	8.8075	1.9062	8.8115
4096	1.9116	5.3643	1.9157	5.3683
exact	1.9345		1.9385	

From the results, we can see that for the first and third column when $n < 512$, the values of $n \times T$ increase and decrease dramatically. This is due to the contribution of the interval which lies on the left hand side of α by using T rule. This can easily be seen graphically from figure 2.5.1 - 2.5.4. But when $n = 512$ and beyond it the values of $n \times T$ coverge to If gradually, since α will lie on one of the end points of the subintervals in this case.

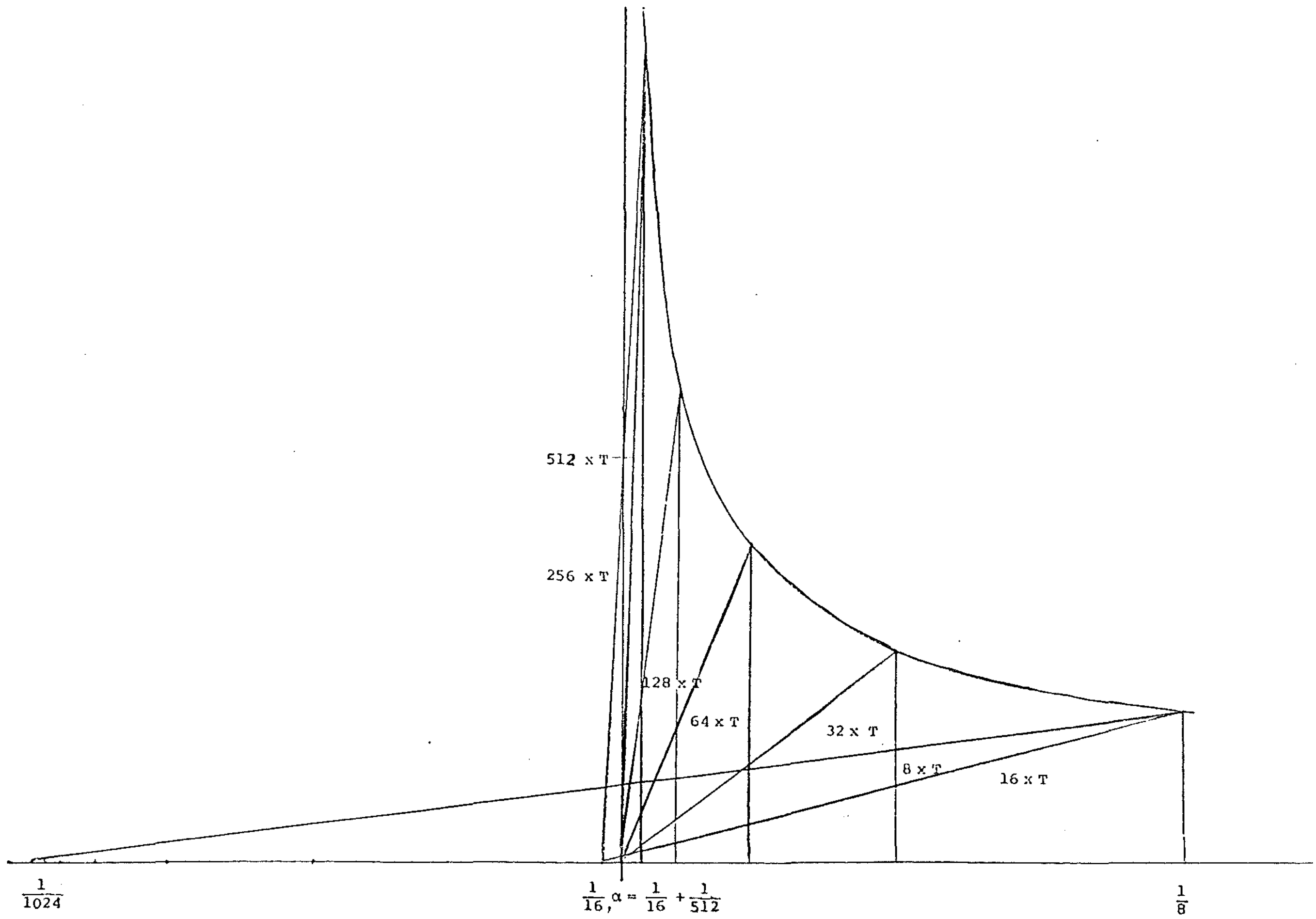

Figure 2.5.1

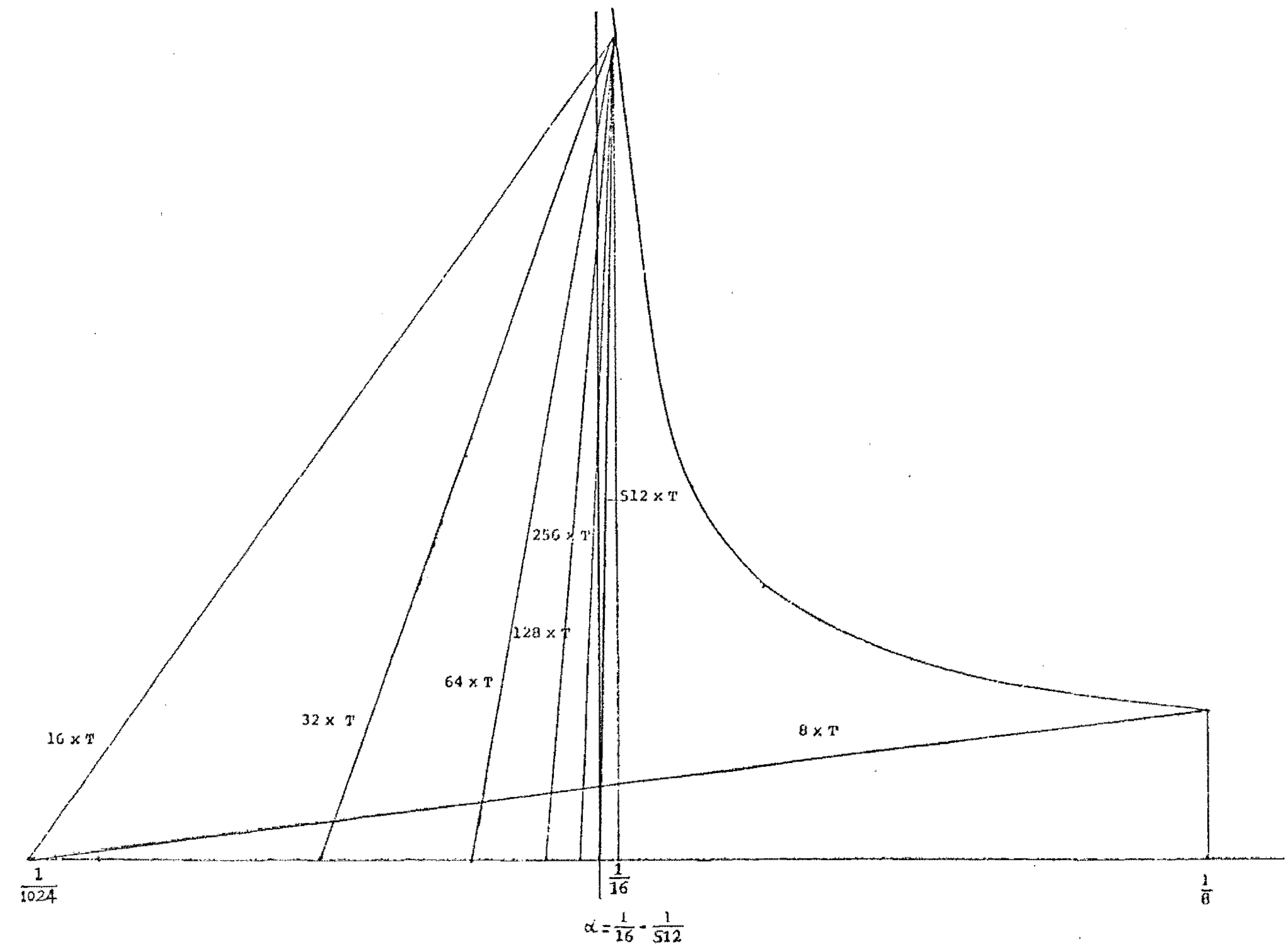

Figure 2.5.2

For $\alpha = \frac{1}{16} \pm \frac{1}{512} - 5 \times 10^{-8}$, the singularity α shifts to the right or left by 5×10^{-8}. It not only contributes some values to the integnant but also induces α away from an end point of a subinterval so the values of n x T increase dramatically.

For $\alpha = \frac{1}{16} + \frac{1}{512} - 5 \times 10^{-8}$

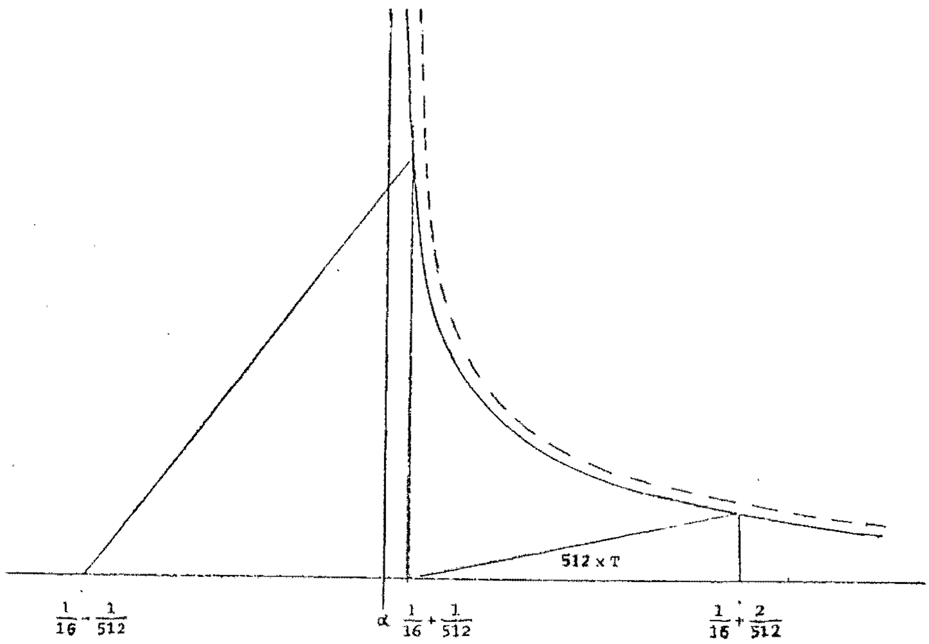

Figure 2.5.3

For $\alpha = \frac{1}{16} - \frac{1}{512} - 5 \times 10^{-8}$

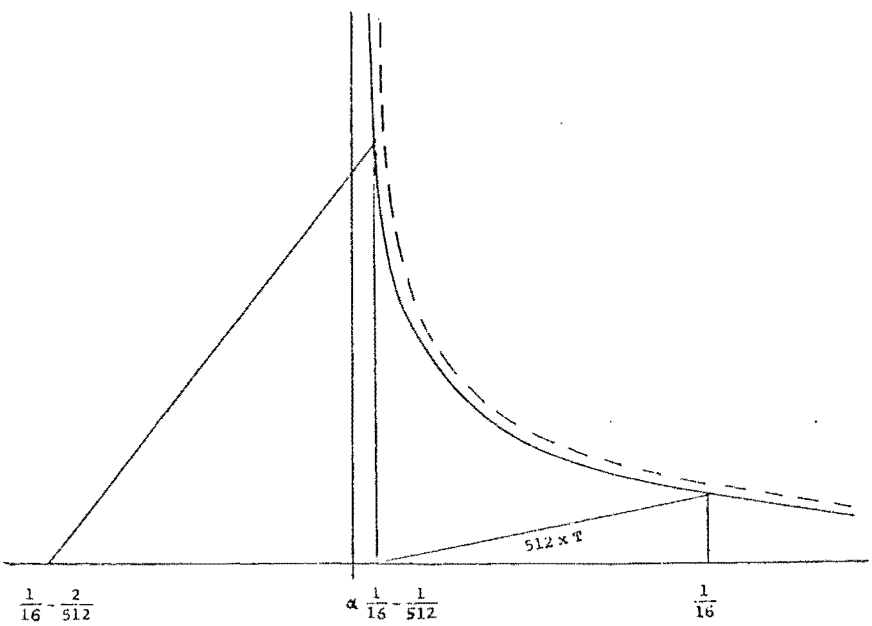

Figure 2.5.4

Now apply n x T to each subinterval which are subdivided from ξ, i.e......$[\alpha, \alpha + \frac{1}{n}]$ $[\alpha + \frac{1}{n}, \alpha + \frac{2}{n}]$.... The results shown as below.

Table 2.5.2

$n \backslash \alpha$	$\frac{1}{16} + \frac{1}{512}$	$\frac{1}{16} + \frac{1}{512} - 5 \times 10^{-8}$	$\frac{1}{16} - \frac{1}{512}$	$\frac{1}{16} - \frac{1}{512} + 5 \times 10^{-8}$
2	0.88668163218	0.88668168735	0.89099027481	0.89099032892
4	1.20093245491	1.20093250707	1.20500319308	1.20500324514
8	1.41738354973	1.41738360147	1.42142147082	1.42142152245
16	1.56920383223	1.56920388396	1.57323992070	1.57323997229
32	1.67627156897	1.67627162067	1.68030633585	1.68030638744
64	1.75191782869	1.75191788039	1.75595228300	1.75595233458
128	1.80539229854	1.80539335023	1.80942667933	1.80942673092
256	1.84320058152	1.84320063323	1.84723494576	1.84723499734
512	1.86993410587	1.86993415757	1.87396846681	1.87396851838
1024	1.88883732025	1.88883737195	1.89287168038	1.89287173195
2048	1.90220385110	1.90220390280	1.90623821101	1.90623826260
4096	1.91165540064	1.91165545233	1.91568976051	1.91568981211
8192	1.91833865143	1.91833870312	1.92237301127	1.92237306286
exact	1.934473443	1.934473494	1.938507802	1.938507854

Note that the convergence, while slow, is monotonic in these cases.

Example 2 (Example 5 in [1]).

$$\int_A^1 f(x)\,dx = 2.0 \qquad f(x) = \begin{cases} \dfrac{1}{\sqrt{x}} & \text{if } x > 0 \\ 0 & \text{if } x \leqslant 0 \end{cases}$$

Here an integral covers a range including 0 with the singularity at 0. As mentioned in [1], for A = -0.5, this is equivalent to a rational singularity while for the other values of A, this is an 'irrational' singularity.

For A = - 0.5 by Simpson rules we have the following results.

Table 2.5.3

n	S	n	S
16	2.06297023	24	1.77748734
32	1.81440591	48	1.84265980
64	2.03148514	96	1.88874368
128	1.90720296	192	1.92132990
256	2.01574257	384	1.94437184
512	1.95360148	768	1.96066495
1024	2.00767129	1536	1.97218592
2048	1.97680074	3072	1.98033247
4096	2.00393564	6144	1.98609296

Since for n = 24, the singularity $\xi = 0$ will fall on the end point of the 8th subinterval and it stays on the end point of a subinterval when n doubles itself. But not for n = 16 x K where K = 1,2...

Now applying S and T to n subintervals subdivided from $\xi = 0$ for other values of A.

Table 2.5.4

S_n \ A	-0.93727082	-0.06272918
2	1.1235524300	1.3510465951
4	1.3805514715	1.5412234050
8	1.5620068842	1.6755996258
16	1.6902936632	1.7706144828
32	1.7810046491	1.8377999394
64	1.8451469087	1.8853072378
128	1.8905023295	1.9188999699
256	1.9225734545	1.9426536191
512	1.9452511646	1.9594499852
1024	1.9612867272	1.9713268095
2048	1.9726255823	1.9797249927
4096	1.9806433635	1.9856634052
8192	1.9863127931	1.9898624965

Table 2.5.5

T_n \ A	-93727082	-0.06272918
2	0.52371285046	0.92023807345
4	0.97359403996	1.24385416526
8	1.27881361845	1.46694367647
16	1.49121007266	1.62344988396
32	1.64052427042	1.73382332040
64	1.74588585904	1.81180578698
128	1.82033164635	1.86693187740
256	1.87295965866	1.90590794927
512	1.91017000566	1.93346720149
1024	1.93648087494	1.95295428918
2048	1.95508526425	1.96673367944
4096	1.96824050299	1.97647716453
8192	1.97754264860	1.98336684456

So from the above results, it can be seen that no matter what the singularity is, rational or irrational, as long as it is located at the right position , $Q_n(f)$ appears to converge to If for both rules.

Example 3 (Example 2 in [7])

$$If = \int_0^1 (x^2 - 0.01)^{-1}\,dx = -\ 1.0033534.$$

a) By Trapezoidal rule.

(i) Singularity is not at the end point of a subinterval.

(ii) Use 10 x n intervals where n = 1,2, . . to ensure the singularity always lies on an end point of a subinterval.

The results are given in Table 2.5.6.

Table 2.5.6

n	(i)		(ii)
2	-22.664141414	10	-2.949494949
4	-6.117677257	20	-1.976000608
8	20.614154589	40	-1.489570856
16	4.099809449	80	-1.246435602
32	-22.623676159	160	-1.124887898
64	-6.107221645	320	-1.064119029
128	-20.616792793	640	-1.033735837
256	4.100470581	1280	-1.018544553
512	-22.623510779	2560	-1.010949002
1024	-6.1071800296	5120	-1.007151231
2048	20.616803115	10240	-1.005252347
4096	4.100473154	20480	-1.004303015
8192	-22.623520283	40960	-1.003828211
16384	-6.107180172	81920	-1.003590789

b) By eight point gauss - Legendie rule (as in [7])

Table 2.5.7

n	(i)		(ii)
1	331.0736718456	10	-1.0033534769
2	15.2521969577	20	-1.0033534869
4	107.5354055160	30	-1.0033534745
8	-17.2586765329	40	-1.0033535020
16	-109.5421124872	50	-1.0033534704
32	15.2519695818	60	-1.0033535083
64	107.5354050928	70	-1.0033535242

The results in (i) are at such variance no conclusion can be made since the singularity is not at the end point of a subinterval but (ii) gives a confident answer since the singularity always lies on the end point of a subinterval.

This technique has also been considered by Harris and Evans in [9]; where they generalised the N - point Gaussian quadrature to cater for end-point singularities. They suggested the choice of subintervals such that the singularity lies on an end-point if it is internal, but they have not really extended the idea to other quadrature rules. They have essentially developed special rules for the Gaussian case. The generalization of the quadrature to deal with the singularity (as in [9]) may improve these results, but this approach has not been developed further at this time.

Example 4

$$\int_0^1 f(x)dx \quad f(x) = \begin{cases} (x-\xi)^\gamma |\log^\beta (x-\xi)| & \xi < x \leqslant 1 \\ 0 & 0 \leqslant x \leqslant \xi \end{cases}$$

(i) $\gamma = -0.75$ $\beta = 1$

(ii) $\gamma = -0.75$ $\beta = 2$

(iii) $\gamma = -0.75$ $\beta = 3$

(iv) $\gamma = -0.75$ $\beta = 4$

Table 2.5.8

For $\xi_1 = \frac{1}{16} + \frac{1}{512} - 5 \times 10^{-8}$

n \ S	(i)	(ii)	(iii)	(iv)
	⋮	⋮	⋮	⋮
4096	11.27623246	56.96898695	356.55062799	2502.02188878
8192	11.82991446	62.62925927	414.18333843	3086.69360400
	⋮	⋮	⋮	⋮
exact	15.62188501	124.9783736	1499.740385	23995.8462

For $\xi_2 = \frac{1}{16} - \frac{1}{152} - 5 \times 10^{-8}$

Table 2.5.9

n \ S	(i)	(ii)	(iii)	(iv)
	⋮	⋮	⋮	⋮
4096	11.27649708	56.96900403	356.55062910	2502.02188890
8192	11.830179076	62.62927636	414.18333953	3086.69360400
	⋮	⋮	⋮	⋮
exact	15.64529233	125.165236	1501.982754	24031.72407

The convergence of the above integral with these particular β are shown in section 2.4 to be very slow. It is necessary that

$n > 10^3$ in (i)

$n > 10^5$ in (ii)

$n > 10^6$ in (iii)

and $n > 10^{15}$ in (iv)

before beginning monotone convergence.

2.6 CONCLUSION

The original investigation of the process of ignoring the singularity by Davis and Rabinowitz [1] has led to extensions and generalizations [6],[8],[10],[11],[13], as well as studies in the rate of convergence and error bounds [3],[4],[5].

In this chapter it has been shown that the location of the singularity does affect the speed of convergence when the technique of ignoring the singularity is applied to an integrand with singularity, whether it is rational or irrational. Thus, this work is a necessary complement to [1] and [13].

Feldstein and Miller [4] state that avoiding the singularity is easier to handle theoretically while ignoring the singularity is easier to program. Rabinowitz [14] prefers to use a quadrature rule which avoids the singularity. However, experience has shown that most of the results favour quadrature rules with an endpoint singularity. These will be illustrated in the next chapter.

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CHAPTER 3

EXTRAPOLATION PROCESSES FOR INTEGRANDS WITH SINGULARITY

3.1 INTRODUCTION

As mentioned at the beginning of Chapter 2, there are a number of methods to deal with singular integrands, $f(x)$, where $f(x)$ is continuous on $[a,b)$ and has a singularity at b. The value, I of the integral is then defined by

$$I = \lim_{\epsilon \to 0} \int_a^{b-\epsilon} f(x)\,dx \qquad (3.1.1)$$

and is assumed to exist.

There are different approaches to the evaluation of this improper integral. The first approach is to transform the improper integral to a proper integral. The second approach is to modify a classical technique for evaluating proper integrals to the case where a singularity occurs. The third approach is to ignore or avoid the singularity (see Chapter 2 and [18]).

Robinson [19] compared fifteen general purpose numerical integrators by using one hundred and ten test integrands from five different types of behaviour of the integrand. One type is a function with one or more singularities within the integration interval. His results show that for those integrators which are reliable and efficient for this type of function most failures occur for functions which have a singularity at an interior point of the range of integration.

The integrals involving endpoint singularities give accurate and reliable results. At points where the function has a infinite value these algorithms assign the value zero. This is equivalent to the process of ignoring the singularity.

The next section gives a brief introduction to some of the numerical quadrature methods which deal with a singular integrand.

To improve the results, some acceleration procedure such as the Romberg method (unmodified and modified), repeated Aitken's Δ^2 process (apply Aitken's Δ^2 process repeatedly), extended Aitken process, the ε-algorithm or rational extrapolation may be used. These are studied in section 3.3. These acceleration processes can be shown to belong to the Neville type extrapolation. The Aitken's Δ^2 processes (repeated and extended) can be viewed as finding a solution to a fixed point problem. In section 3.4, this approach is extended to the ε-algorithm, and can be shown to give the accelerated value with error of any order k. This chapter ends with some numerical results and conclusions.

3.2 NUMERICAL QUADRATURE FOR AN INTEGRAND WITH ENDPOINT SINGULARITY.

Numerical quadrature formulas for an integrand with endpoint singularity include linear and nonlinear techniques.

For linear quadrature, Harris and Evans [6] modified a 10 point Gauss rule, giving a new set of weights and abscissae such that the formula is exact for polynomials of order up to eleven or less combined with logarithmic, inverse square root, inverse fourth root and inverse three fourth root endpoint singularities. Stenger [27] [28] gives a quadrature rule which is a transformation based on the Trapezoidal formula. It has been shown to give exponential convergence in some cases when the singularity is ignored.

For non-linear quadrature, Sidi [24] used the results of nonlinear transformations - t,u,v transformations [11] to modify numerical quadrature formulas for weight functions with algebraic and/or logarithmic endpoint singularities. He compares these with Gaussian rules and finds that they are simpler to compute and practically as efficient as the corresponding Gaussian rules. Werner and Wuytack [29] give techniques which are based on the use of Spline approximation and Pade approximation. They compare these methods with some other methods and claim that they are competitive with an adaptive Gaussian quadrature scheme.

Squire [25] [26] did a comparison of Harris and Evans' modified 10 point Gaussian rule, Stenger's quadrature and Werner and Wuytack's nonlinear techniques. He concluded that the appropriate linear quadrature can handle an integrand with endpoint singularity more effectively than the nonlinear method.

Sack [21] gives a critical comment on Stenger's quadrature. He agrees that the rules have simplicity and generality but claims that the rate of convergence is rather slow. He points out that an improvement of efficiency can be achieved by acceleration procedures such as repeated application of the Aitken Δ^2 process. Werner and Wuytack [29] also give a technique for using extrapolation to improve the numerical results. This technique in fact is the same as the repeated Aitken Δ^2 process. It will be explained in the next section.

3.3 THE EXTRAPOLATION PROCEDURES AND ASYMPTOTIC ERROR EXPANSION.

A brief description of some of the extrapolation processes are given below.

(a) The classical unmodified Romberg method.

If $f \in C^{2k+1}[a,b]$, then

$$If = \int_a^b f(x)\,dx \tag{3.3.1}$$

can be approximated by the trapezoidal rule

$$T_0^k = h_k \sum_{j=0}^{2^k}{}'' f(a + jh_k) \text{ where } h_k = {}^{(b-a)}/2^k$$

where $\sum''$ indicates that half the contribution is included from each endpoint.

The error, $E(h,f) = If - T_0^k$, can be expressed using the Euler-Maclaurin formula in the form

$$E(h,f) \sim a_1h^2 + a_2h^4 + \ldots + a_kh^{2k} + O(h^{2k+1}),\ h \to 0. \tag{3.3.2}$$

where a_i are constants formed from the Bernoulli numbers and the derivatives of $f(x)$ at the end points.

The classical Romberg method combines T_0^0, T_0^1 . . . linearly and the successive error terms in $E(h,f)$ can be eliminated according to

$$T_m^{\ k} = \frac{4^m T_{m-1}^{k+1} - T_{m-1}^{k}}{4^m - 1} \qquad m = 1,2,\ldots \qquad (3.3.3)$$

This can be generalized to

$$T_m^{\ k} = \frac{h_k^2 \, T_{m-1}^{k+1} - h_{k+m}^2 \, T_{m-1}^{k}}{h_k^2 - h_{k+m}^2} \quad \text{where } h_k = {}^{(b-a)}/n_k \qquad (3.3.4)$$

Different sequences $\{n_k\}$ have been used to accelerate convergence [2], [3].

Oliver [16] did a comparison of various methods based on polynomial extrapolation for the definite integrals. He concluded that for a general purpose procedure extrapolation of the trapezoidal rule, using a sequence favoured by Burlirsch [2] gives maximum accuracy.

(b) <u>Modified Romberg method.</u>

However, the Euler-Maclaurin summation formula for the error expansion E(h,f) (3.3.2) is not suitable for numerical computation if f(x) has a singularity. Navot [13], [14] and Lyness and Ninham [12], [15] have generalized the asymptotic expansions suitable in such case. When f(x) has a singularity at an endpoint (3.3.2) is replaced by

$$E(h,f) \sim a_1 h^{\alpha_1} + a_2 h^{\alpha_2} + \ldots + a_k h^{\alpha_k} + O(h^{\alpha_{k+1}}) \quad 0<\alpha_1<\alpha_2<\ldots \quad (3.3.5)$$

If $\alpha_1 \neq 2$ then the use of (3.3.3) or (3.3.4) in this case gives $If - T_k^0 = O(h^{\alpha_1})$ and the convergence of T_k^0 is at the same rate as the trapezoidal rule $T_0^{\ k}$.

Fox [5] gives an account for the h^{α_i} terms in (3.3.5). For functions with an unbounded first derivative at an endpoint (lower limit is taken here), he shows that the contribution to the error in the trapezoidal and Simpson's rule $E_T(h)f_0$ and $E_S(h)f_0$, for a sufficiently small interval h, comes from the lower limit in the forms

$$E_T(h)f_0 = \left(\frac{1}{12}h^2D - \frac{1}{12}h^3D^2 + \frac{29}{720}h^4D^3 \cdot \cdot \cdot\right)f_1 \qquad (3.3.6)$$

$$E_S(h)f_0 = \left(\frac{1}{180}h^4D^3 - \frac{1}{180}h^5D^4 + \frac{2}{945}h^6D^5 . . .\right)f_1 \qquad (3.3.7)$$

where D^i is the ith derivative of f(x). These terms then added to the usual series of powers h^2, h^4, h^6... for trapezoidal rule and h^4, h^6, h^8.. for Simpson's rule respectively which are derived at the upper limit if the integrand is completely well-behaved except at a. For those functions with a singularity in the integrand at one or both endpoints, Fox prefers a formula which does not include these points. He proposes the use of composite midpoint rule and the term embodied in the error is

$$E_u(h)f_0 = \left(-\frac{1}{6}h^2D + \frac{1}{6}h^3D^2 - \frac{23}{360}h^4D^3 + \cdot \cdot \cdot\right)f_1 \qquad (3.3.8)$$

together with the standard even powers of h if the function is well-behaved.

For example if $I = \int_0^1 x^{\frac{1}{2}}dx$, then

$$I - T(h) = a_1h^{3/2} + a_2h^2 + a_3h^4 + \ldots$$

For a function with a logarithmic endpoint singularity the error expansion is more complicated [13].

Shanks [23] gives a simple and economic technique to eliminate these lower order terms in this error expansion.

It is equally applicable for more complicated error terms with repeated occurrence of the $\ln h$ term. For example,

If $I = -\int_0^1 x \ln^3 x \, dx$ then

$$I - T(h) = ah^2 + bh^2 \ln h + ch^2 \ln^2 h + dh^2 \ln^3 h + eh^4 + fh^6 + \cdots$$

The error terms can be eliminated by using the modification of (3.3.3)

$$T_m^{k} = \frac{2^{\alpha_m} T_{m-1}^{k+1} - T_{m-1}^{k}}{2^{\alpha_m} - 1} \qquad (3.3.9)$$

with $\alpha_m = 2, 2, 2, 2, 4, 6, . . .$

(c) Aitken's Δ^2 process.

If α_m is not known, Werner and Wuytack [29] suggest that these can be approximated numerically. Assume an expansion of the form

$$I - Q(h) = \sum_{i=0}^{\infty} a_i h^{\alpha_i} \quad \text{with } a_0 \neq 0 \qquad (3.3.10)$$

where $Q(h)$ is an approximation for the integral I in (3.1.1) and the a_i and α_i are unknowns. Consider $Q(h)$, $Q(\frac{h}{2})$ and $Q(\frac{h}{4})$. α_0 can be approximated by

$$2^{\alpha_0} = \frac{Q(\frac{h}{2}) - Q(h)}{Q(\frac{h}{4}) - Q(\frac{h}{2})}$$

Then $I = Q(\frac{h}{4}) + \frac{Q(\frac{h}{4}) - Q(\frac{h}{2})}{2^{\alpha_0} - 1}$

This is the well known Aitken's Δ^2 process which uses three successive estimates to eliminate the lowest order term in the error. When α_0 is found, a similar technique can be used to find $\alpha_1, \alpha_2 \ldots$; that is to apply Aitken's Δ^2 process repeatedly.

(c1) Repeated Aitken's Δ^2 process.

The Aitken's Δ^2 process, used on the converging sequence $\{x_i\}$, can be considered as the iteration

$$x_{i+1} = \phi(x_i)$$

which converges to a solution $x = X$ of a function $f(x) = \phi(x) - x = 0$.

Let the error in x_i be E_i.

$x_i = X + E_i$.

Suppose $\phi(x)$ is analytic around X. Then

$$x_1 = \phi(x_0)$$

$$= X + a_1E_0 + a_2E_0^2 + a_3E_0^3 + \ldots$$

and $x_2 = \phi(x_1)$

$$= X + a_1E_1 + a_2E_1^2 + a_3E_1^3 + \ldots$$

where $E_1 = a_1E_0 + a_2E_0^2 + a_3E_1^3 + \ldots$

and $a_i = \phi^i(X)/i!$

Convergence is then assumed if $|\phi'(x)|<1$ in some neighbourhood of X, which implies $|a_1|<1$.

Combining these three first order approximations x_0, x_1 and x_2, a second-order approximation, x_{12}, is obtained

$$x_{12} = X + a_{22}E_0^2 + a_{32}E_0^3 + \ldots$$

with an asymptotic error constant

$$a_{22} = -\frac{a_1 a_2}{1-a_1}$$

and the Aitken value

$$x_{12} = \frac{x_1^2 - x_0 x_2}{2x_1 - x_0 - x_2} = x_0 - \frac{(\Delta x_0)^2}{\Delta^2 x_0}$$

where $\Delta x_0 = x_1 - x_0$ and $\Delta^2 x_0 = x_2 - 2x_1 + x_0$.

Using the same process repeatedly, the Aitken values can be obtained column by column and can be written in the following array

$$\begin{array}{llll}
x_{0,1} & & & \\
x_{1,1} & x_{1,2} & & \\
x_{2,1} & x_{2,2} & x_{2,3} & \\
x_{3,1} & x_{3,2} & \vdots & \cdot \\
x_{4,1} & \vdots & & \\
\vdots & & &
\end{array}$$

where $\{x_{i,1}\} = \{x_i\} \quad i = 0,1,2...$

Figure 3.3.1.

This repeated process can be expressed in the form

$$x_{j,k+1} = x_{j-1,k} - \frac{(x_{j,k} - x_{j-1,k})^2}{x_{j+1,k} - 2x_{j,k} + x_{j-1,k}}$$

$$= \frac{x_{j+1,k} - d_{k+1}^j \, x_{j,k}}{1 - d_{k+1}^j} \qquad (3.3.11)$$

where $$d_{k+1}^j = \frac{x_{j+1,k} - x_{j,k}}{x_{j,k} - x_{j-1,k}} \qquad (3.3.12)$$

(c2) Extended Aitken process.

Overholt [17] observed that any first-order approximation gives a second-order formula and he extended the Aitken's Δ^2 process in the following way.

Suppose that the first k+1 members of the sequence $\{x_i\}$ used in a certain function, ϕ_k, to give an X-approximation of order k. Then

$$x_{1,k} = \phi_k(x_{0,1}, x_{1,1} \dots x_{k,1})$$
$$= X + a_{k,k}E_0^{\ k} + a_{k+1,k}E_0^{\ k+1} \dots \text{ where } a_{kk} \neq 0 .$$

The next value is

$$x_{2,k} = X + a_{k,k}E_1^{\ k} + a_{k+1,k}E_1^{\ k+1} \dots$$

where $E_1^{\ k} = a_1^{\ k}E_0^{\ k} + ka_1^{\ k-1}a_2E_0^{\ k+1} \quad \dots$

Then the accelerated value $x_{1,k+1}$ of order k+1 is

$$x_{1,k+1} = x_{2,k} + \frac{a_1^{\ k}}{1-a_1^{\ k}}(x_{2,k}-x_{1,k})$$

where a_1 can be approximated by

$$a_1 = \frac{x_{1+k,1} - x_{k,1}}{x_{k,1} - x_{k-1,1}}$$

The array is the following

$$\begin{array}{lllll}
x_{0,1} & & & & \\
x_{1,1} & x_{1,2} & x_{1,3} & x_{1,4} & \cdots \\
x_{2,1} & x_{2,2} & x_{2,3} & \vdots & \\
x_{3,1} & x_{3,2} & \vdots & \cdot & \\
x_{4,1} & \vdots & \cdot & & \\
\vdots & & & &
\end{array}$$

Figure 3.3.2

In general

$$x_{j,k} = X + a_{kk}E_{j-1}^{k} + a_{k+1,k}E_{j-1}^{k} + \dots$$

and $$E_j^k = a_1^k E_{j-1}^k + ka_1^{k-1} a_2 E_{j-1}^{k+1} + \dots \qquad (3.3.13)$$

The recursive formula can be written as

$$x_{j,k+1} = x_{j+1,k} + \frac{(\tilde{d}_{k+1}^{j})^k}{1-(\tilde{d}_{k+1}^{j})^k}(x_{j+1,k} - x_{j,k})$$

$$= \frac{x_{j+1,k} - (\tilde{d}_{k+1}^{j})^k x_{j,k}}{1 - (\tilde{d}_{k+1}^{j})^k} \qquad (3.3.14)$$

where $$\tilde{d}_{k+1}^{j} = \frac{x_{j+k,1} - x_{j+k-1,1}}{x_{j+k-1,1} - x_{j+k-2,1}} \qquad (3.3.15)$$

(d) The ε-algorithm.

An important generalization of (c) known as the ε-algorithm is due to Shanks [22] and Wynn [30].

The fundamental relationship of the ε-algorithm is

$$(\varepsilon_{k+1}^{j} - \varepsilon_{k-1}^{j+1})(\varepsilon_{k}^{j+1} - \varepsilon_{k}^{j}) = 1 \qquad (3.3.16)$$

In applications, this relationship is rearranged to give

$$\varepsilon_{k+1}^{j} = \varepsilon_{k-1}^{j+1} + (\varepsilon_{k}^{j+1} - \varepsilon_{k}^{j})^{-1} \qquad j, k = 0,1 \dots$$

with $$\varepsilon_{-1}^{j} = 0 \qquad j = 1,2 \dots$$

$$\varepsilon_{0}^{j} = x_{j,1} \qquad j = 0,1 \dots$$

where $x_{j,1}$ is a member of a slowly convergent (or divergent) sequence. The approximant of $x_{j,1}$ is given by ε_{2k}^{j}. The quantities ε_{2k+1}^{j} which are only the intermediate results, can be eliminated from the rule of the ε-algorithm [32].

$$(\varepsilon_{2k}^{j-1} - \varepsilon_{2k}^{j})^{-1} + (\varepsilon_{2k}^{j+1} - \varepsilon_{2k}^{j})^{-1} = (\varepsilon_{2k-2}^{j+1} - \varepsilon_{2k}^{j})^{-1} + (\varepsilon_{2k+2}^{j-1} - \varepsilon_{2k}^{j})^{-1}$$

$$\text{for} \quad k = 0,1,2,\ldots \quad j = 1,2,3,\ldots \qquad (3.3.17)$$

$$\text{with } \varepsilon_{-2}^{j} = \infty$$

$$\text{and} \quad \varepsilon_{0}^{j} = x_j$$

ε_k^j can be set out in the array shown in figure 3.3.3.

$$\begin{array}{cccccc}
 & \varepsilon_0^0 & & & & \\
\varepsilon_{-1}^1 & & \varepsilon_1^0 & & & \\
 & \varepsilon_0^1 & & \varepsilon_2^0 & & \\
\varepsilon_{-1}^2 & & \varepsilon_1^1 & & \cdot & \\
 & \varepsilon_0^2 & & \varepsilon_2^1 & \cdot & \cdot \\
\varepsilon_{-1}^3 & & \varepsilon_1^2 & \cdot & & \\
 & \varepsilon_0^3 & \cdot & \cdot & & \\
\cdot & & \cdot & & & \\
\cdot & \cdot & & & &
\end{array}$$

Figure 3.3.3

If $2n+1$ x_j s are given, with k constant for the columns and j constant for the upper diagonals, then the sequences ε_0^j $(j = 0,1,2\ldots 2n)$, $\varepsilon_{2k}^j (k=0,1,2\ldots(2n-2))$ successively give better results than $\{x_j\}$. The convergence and stability of this algorithm can be found in [31].

Macdonald [20] showed that ε_{2k+2}^{j-1} can be expressed in terms of ε_{2k}^{j-1}, ε_{2k}^{j}, ε_{2k}^{j+1} and the two values ε_{2k-1}^{j+1} and ε_{2k-1}^{j} in the preceding column. The transformation is

$$\varepsilon_{2k+2}^{j-1} = \frac{D_{2k+2}^{j-1}}{1+G_{2k+2}^{j-1}} + \left(\frac{G_{2k+2}^{j-1}}{1+G_{2k+2}^{j-1}}\right)\varepsilon_{2k}^{j} \tag{3.3.18}$$

where

$$D_{2k+2}^{j-1} = \varepsilon_{2k}^{j+1} - \frac{(\varepsilon_{2k}^{j+1} - \varepsilon_{2k}^{j})^2}{\varepsilon_{2k}^{j+1} - 2\varepsilon_{2k}^{j} + \varepsilon_{2k}^{j-1}} \tag{3.3.19}$$

and $$G_{2k+2}^{j-1} = (\varepsilon_{2k-1}^{j+1} - \varepsilon_{2k-1}^{j})(D_{2k+2}^{j-1} - \varepsilon_{2k}^{j}) \tag{3.3.20}$$

where $G_{2k+2}^{j-1} = 0$,(3.3.17) shows that $\varepsilon_{2k+2}^{j-1} = D_{2k+2}^{j-1}$ which reduces to the Aitken's Δ^2 process (3.3.11). (3.3.18) can be rearranged in terms of the elements in the even column, i.e., ε_{2k}^{j-1}, ε_{2k}^{j}, ε_{2k}^{j+1} and ε_{2k-2}^{j+1}, can be expressed by a similar expression to (3.3.11) and (3.3.14). This gives another expression of (3.3.17). Since D_{2k+2}^{j-1} is the Aitken's Δ^2 process, it can be written as

$$D_{2k+2}^{j-1} = \frac{\varepsilon_{2k}^{j+1} - d_{2k+2}^{j+k}\,\varepsilon_{2k}^{j}}{1 - d_{2k+2}^{j+k}}$$

where $$d_{2k+2}^{j+k} = \frac{\varepsilon_{2k}^{j+1} - \varepsilon_{2k}^{j}}{\varepsilon_{2k}^{j} - \varepsilon_{2k}^{j-1}}$$

Then substitute the above expression into (3.3.18)

$$\varepsilon_{2k+2}^{j-1} = \frac{\varepsilon_{2k}^{j+1} - \bar{d}_{2k+2}^{j+k}\,\varepsilon_{2k}^{j}}{1 - \bar{d}_{2k+2}^{j+k}} \tag{3.3.21}$$

where $$\bar{d}_{2k+2}^{j+k} = d_{2k+2}^{j+k} - (1-d_{2k+2}^{j+k})\,G_{2k+2}^{j-1}$$

Substituting for G_{2k+2}^{j-1} from (3.3.19) and (3.3.20) gives

$$\bar{d}^{j+k}_{2k+2} = d^{j+k}_{2k+2} - (\varepsilon^{j+1}_{2k-1} - \varepsilon^{j}_{2k-1})(\varepsilon^{j+1}_{2k} - \varepsilon^{j}_{2k})$$

If $\varepsilon^{j+1}_{2k-1} - \varepsilon^{j}_{2k-1} \neq 0$ then from (3.3.16),

$$\bar{d}^{j+k}_{2k+2} = d^{j+k}_{2k+2} - \frac{\varepsilon^{j+1}_{2k} - \varepsilon^{j}_{2k}}{\varepsilon^{j}_{2k} - \varepsilon^{j+1}_{2k-2}}$$

$$= \frac{\varepsilon^{j-1}_{2k} - \varepsilon^{j+1}_{2k-2}}{\varepsilon^{j}_{2k} - \varepsilon^{j+1}_{2k-2}} \; d^{j+k}_{2k+2} \qquad (3.3.22)$$

Since the even columns ε^{j}_{2k} give the accelerated values of $\{x_{j,1}\}$ it can be written as

$$\varepsilon^{j}_{2k} = x_{j+k,k} \qquad \begin{array}{l} k = 1,2 \ldots \\ j = 0,1,2\ldots \end{array}$$

Then (3.3.21) can be expressed as

$$x_{j+k,k+1} = \frac{x_{j+k+1,k} - \bar{d}^{j+k}_{k+1}\, x_{j+k,k}}{1 - \bar{d}^{j+k}_{k+1}} \qquad \begin{array}{l} k = 1,2\ldots \\ j = 0,1,2\ldots \end{array}$$

and this can be simplified to

$$x_{j,k+1} = \frac{x_{j+1,k} - \bar{d}^{j}_{k+1}\, x_{j,k}}{1 - \bar{d}^{j}_{k+1}} \qquad \begin{array}{l} k = 1,2\ldots \\ j = k,k+1\ldots \end{array} \qquad (3.3.23)$$

where $$\bar{d}^{j}_{k+1} = \frac{x_{j-1,k} - x_{j,k-1}}{x_{j,k} - x_{j,k-1}} \cdot \frac{x_{j+1,k} - x_{j,k}}{x_{j,k} - x_{j-1,k}} \qquad (3.3.24)$$

(e) Rational extrapolation.

Bulirsch and Stoer [3] developed a nonlinear method for accelerating the convergence of a sequence Q(h) (3.3.10). The approximant Q(h) of I is now approximated by a rational function $R^i_{\mu,\nu}(h)$. For an expansion in terms of h^2

$$R^i_{\mu,\nu}(h^2) = \frac{a^i_0 + a^i_1 h^2 + \ldots + a^i_\mu h^{2\mu}}{b^i_0 + b^i_1 h^2 + \ldots + b^i_\nu h^{2\nu}}$$

The recursion formulas analogous to (3.3.4) are rather complicated, but can be simplified by choosing $\mu = [m/2]$ and $\nu = m - [m/2]$ and writing $R^i_{\mu,\nu} = R^i_m$. In this case the formulas become

$$R^i_m = \frac{R^{i+1}_{m-1} - \hat{d}^i_m R^i_{m-1}}{1 - \hat{d}^i_m} \tag{3.3.25}$$

with $R^i_{-1} = 0$

$R^i_0 = Q(h_i)$.

where $$\hat{d}^i_m = \left(\frac{h_{i+m}}{h_i}\right)^2 \frac{R^{i+1}_{m-1} - R^{i+1}_{m-2}}{R^i_{m-1} - R^{i+1}_{m-2}} \tag{3.3.26}$$

An algorithm for generalized rational extrapolation will be given in the next chapter.

Havie [7] generalized the Neville extrapolation to an expansion for which the extrapolation coefficients used in the calculation of the elements in the related extrapolation table are not known. He considered the expansion

$$Q(h) = Q(0) + \sum_{m=1}^{n} a_m e_m(h) + R_n(h) \qquad (3.3.27)$$

where $e_j(h)$ $j = 1,2\ldots$ are known functions satisfying $\lim_{h\to 0} \dfrac{e_{m+1}(h)}{e_m(h)} = 0$ and $R_n(h) = 0(e_{n+1}(h))$ is the error term. $Q(0)$, $a_1, a_2 \ldots a_n$ are unknowns and $Q(h)$ can be calculated for a sequence of steplengths $h_0 > h_1 > h_2 > \ldots > 0$. The unknowns $a_1, a_2 \ldots a_n$ can be eliminated successively by computing the lower triangular table

$$\begin{array}{lllll}
Q_0^0 & & & & \\
Q_0^1 & Q_1^0 & & & \\
Q_0^2 & Q_1^1 & Q_2^0 & & \\
\cdot & \cdot & \cdot & \cdot & \\
\cdot & \cdot & \cdot & \cdot & \\
Q_0^n & Q_1^{n-1} & Q_2^{n-2} & \cdots & Q_n^0
\end{array}$$

Figure 3.3.4

With the elements defined by Neville's algorithm

$$Q_m^{\ell} = \frac{Q_{m-1}^{\ell+1} - d_m^{\ell}\, Q_{m-1}^{\ell}}{1 - d_m^{\ell}} \qquad m > 0 \qquad (3.3.28)$$

and starting with $Q_0^{\ell} = Q(h_{\ell})$ where the extrapolation coefficients d_m^{ℓ} are defined by

$$d_m^{\ell} = \frac{E_{m-1,m}^{\ell+1}}{E_{m-1,m}^{\ell}} \qquad (3.3.29)$$

$$E_{m,j}^{\ell} = \frac{E_{m-1,j}^{\ell+1} - d_m^{\ell}\, E_{m-1,j}^{\ell}}{1 - d_m^{\ell}} \qquad (3.3.30)$$

with $E^{\ell}_{0,j} = e_j(h_\ell)$. Q^{ℓ}_m is related to $Q(0)$ through the expansion

$$Q^{\ell}_m = Q(0) + \sum_{j=m+1}^{n} a_j E^{\ell}_{m,j} + R^{\ell}_m$$

The error elements satisfy the Neville's algorithm if the Q-elements are replaced by the R-elements with $R^{\ell}_0 = R_n(h_\ell)$.

Comparing the elements Q^{ℓ}_m, which are obtained from the extrapolation processes (a) - (e), to the expansion (3.3.27), we note that they have a recursive relation similar to (3.3.28) - (3.3.30). It is well known that (a) and (c) are of this type. The extrapolation coefficients d^{ℓ}_m can be obtained from (3.3.29). (e) is similar to this type but the extrapolation coefficients d^{ℓ}_m are approximated by nonlinear transformation (3.3.24).

For (a) and (b), two successive terms in a column are needed for extrapolation in (3.3.3) and (3.3.4) provided d^{ℓ}_m is known. If d^{ℓ}_m is not known, for example (c1), a third term is needed in the same column in (3.3.11). For (c2), since the approximation of d^{ℓ}_m based on its first approximation three successive terms are needed to give the first approximation of d^{ℓ}_m in the first column; the rest need only two successive terms (see (3.3.14)). For (d) three successive terms in a column and a term in the preceding column are needed and (e) is the same as (d), but instead of three successive terms, only two terms are needed.

3.4 COMPARISON AND ERROR ANALYSIS OF SOME EXTRAPOLATION PROCESSES

The comparison of the extrapolation processes (a), (b), (c1) and (d) and the comparison of (a), (d) and (e) are given in [4] and [10] respectively. Their conclusions are that for well-behaved integrands, (a) and (e) give reasonably effective results. For functions with endpoint singularities (b) gives the best results provided all the exponents in the asymptotic error expansion are known. Otherwise (c1) gives better results than (a) and (e). In the case of functions with logarithmic endpoint singularities, the error expansion is more complicated and (d) gives better results than (c1) but not as good as (b).

The extrapolation processes (c1), (c2) and (d) can be considered as finding a solution to a fixed point problem, i.e., considering $x_{i,k}$ as a function of $x_{i-1,k}$. $x_{i,k} = \phi_k(x_{i-1,k})$, a one-point iterating function of order k with the asymptotic error constant $a_{k,k}$ given. Overholt [ ]7] gave the (k + 1)th order approximation $x_{j,k+1}$ of X by the extended Aitken method (3.3.13) with an asymptotic error constant

$$a_{k+1,k+1} = \frac{a_1^{\;k}}{1-a_1^{\;k}} \{- \; k\, a_2 a_{k,k} + (a_1 - 1) a_{k+1,k}\}$$

This expression appears to be in error and should be expressed as

$$a_{k+1,k+1} = \frac{a_1^{\;k-1}}{1-a_1^{\;k}} \left[k\, a_2\{1 - a_1^{\;k-1}(1+a_1)\}a_{k,k} + a_1(a_1-1)a_{k+1,k}\right] \tag{3.4.1}$$

Since from (3.3.15) $\tilde{d}^{\,j}_{k+1}$ (denoted as τ_{j+k} in [17]) can be expanded in terms of a_1 via (3.3.13).

$$\tilde{d}^{\,j}_{k+1} = a_1 + \alpha_1 E_{j-1} + \ldots$$

$\tilde{d}^{\,j}_{k+1}$ is the first order approximation of a_1 with $\alpha_1 = (1 + a_1)^{k-1} a_1 a_2$.

Substituting this and (3.3.13) in (3.3.14) gives $x_{j,k+1}$ with $a_{k+1,k+1}$ which is given by (3.4.1).

The repeated Aitken's Δ^2 process, extended Aitken process and the ε-algorithm give the same approximation $x_{j,2}$ where $j = 1, 2 \ldots$ on the second column of their arrays (Figure 3.3.1 - 3.3.3).

$$x_{j,2} = X + a_{22} E^2_{j-1} + a_{32} E^3_{j-1} + \ldots \qquad (3.4.2)$$

with $$a_{22} = \frac{-a_1 a_2}{1-a_1}, \quad a_{32} = - a_1 a_3 \frac{1+a_1}{1-a_1} - a_2^{\,2} \frac{1+a_1^{\,2}}{(1-a_1)^2}$$

Using (3.3.11), (3.3.14), (3.3.21) and (3.4.2) again, it follows

$$x_{j,3} = X + a_{33} E^3_{j-2} + \ldots \qquad j = 2,3,\ldots$$

with $$a_{33} = \left\{\frac{2a_1^{\,3} a_2}{1-a_1^{\,2}}(1-a_1 - a_1^{\,2})\, a_{22} - \frac{a_1^{\,4}}{1+a_1} a_{32}\right\} a_1$$

$$= \left(- \frac{a_1^{\,4} a_2^{\,2}}{1-a_1} \cdot \frac{1-3a_1}{1-a_1} + \frac{a_1^{\,5} a_3}{1-a_1}\right) a_1 \quad \text{for extended Aitken process} \qquad (3.4.3)$$

$$a_{33} = \left(- \frac{2a_1^{\,3} a_2}{1-a_1^{\,2}} a_{22} + \frac{a_1^{\,4}}{1+a_1} a_{32}\right) \frac{1}{1+a_1}$$

$$= \left(\frac{a_1^{\,4} a_2^{\,2}}{1-a_1} - \frac{a_1^{\,5} a_3}{1-a_1}\right) \frac{1}{1+a_1} \quad \text{for repeated Aitken's } \Delta^2 \text{ process} \qquad (3.4.4)$$

$$a_{33} = a_1^2 a_{22}^2 + \left(- \frac{2a_1^3 a_2}{1-a_1^2} a_{22} + \frac{a_1^4}{1+a_1} a_{32}\right) \frac{1}{1+a_1}$$

$$= \left\{\frac{2a_1^4 a_2^2 - a_1^5 a_3(1-a_1)}{(1-a_1)^2}\right\} \frac{1}{1+a_1} \quad \text{for the } \varepsilon\text{-algorithm} \tag{3.4.5}$$

Hence these three processes give an approximation $x_{j,3}$ to X of order three with slightly different coefficients a_{33}.

Now the same assumption is made as in the extended Aitken process. $x_{j,k}$ for $k = 2,3,\ldots,$ $j = k-1,k,\ldots$ is the k th column of the approximation of $\{x_{j,1}\}$ $j = 0,1,2,\ldots$ obtained by the repeated Aitken's Δ^2 process and the ε-algorithm. Assume that these $x_{j,k}$ give an X approximation of order k+1.

Write

$$x_{j,1} = X + E_j \qquad j = 0,1,2,\ldots$$

where

$$E_j = a_1 E_{j-1} + a_2 E_{j-1}^2 + a_3 E_{j-1}^3 + \ldots$$

and

$$x_{j,k+1} = X + a_{k+1,k+1} E_{j-k}^{k+1} + a_{k+2,k+1} E_{j-k}^{k+2} + \ldots$$

$$\text{for } k = 1,2,\ldots \quad j = k,k+1,\ldots \tag{3.4.6}$$

Then by (3.3.11) and (3.3.12), using the same method as in deriving (3.4.1)

$$a_{k+1,k+1} = \frac{a_1^{2k-1}(1-a_1)}{(1-a_1^k)^2} \left\{-k a_2 a_{k,k} + a_1(1-a_1)\, a_{k+1,k}\right\}$$

$$\text{for repeated Aitken's } \Delta^2 \text{ process.} \tag{3.4.7}$$

by (3.3.23) and (3.3.24)

$$a_{k+1,k+1} = \frac{a_{k,k}^2}{a_{k-1,k-1}} a_1^2 + \frac{a_1^{2k-1}(1-a_1)}{(1-a_1^k)^2} \left\{-k a_2 a_{k,k} + a_1(1-a_1) a_{k+1,k}\right\}$$

$$\text{for the } \varepsilon\text{-algoritm.} \tag{3.4.8}$$

It is not easy to tell which one is better without knowing some information about the iteration function of the given sequence. From numerical experiments, the repeated Aitken's Δ^2 process is better than the extended Δ^2 process. The ε-algorithm is probably the best. In some cases such as an oscillating sequence, some of the columns obtained from repeated Aitken's Δ^2 process are slightly faster than the ε-algorithm, but the ε-algorithm will catch up later.

3.5 NUMERICAL RESULTS

The approximation of the following integrals with endpoint singularities or the first derivatives with endpoint singularities are approximated by Trapezoidal rule T_n (ignoring the singularities) then accelerated by (i) Modified Romberg method (ii) extended Δ^2 process (iii) repeated Δ^2 process and (iv) the ε-algorithm.

Table 3.5.1

a) $\int_0^1 x^{-\frac{1}{2}} dx = 2.$

(i)

n							
1	0.957106781						
2	1.267228525	2.015928645					
4	1.483036302	2.004042364	2.000080271				
8	1.634748652	2.001014665	2.000005432	2.000000443			
16	1.741802668	2.000253925	2.000000346	2.000000006	2.000000000		
32	1.817445514	2.000063499	2.000000023	2.000000002	2.000000002	2.000000002	
64	1.870919134	2.000015873	2.000000000	1.999999996	1.999999996	1.999999996	
128	1.908727207	2.000003970	2.000000002	2.000000002	2.000000002	2.000000002	
256	1.935460679	2.000000990	1.999999996	1.999999996	1.999999996	1.999999996	
512	1.954363881	2.000000248	2.000000000	2.000000001	2.000000001	2.000000001	
1024	1.967730409	2.000000062	2.000000000	2.000000000	2.000000000	2.000000000	
2048	1.977181958	2.000000016	2.000000000	2.000000000	2.000000000	2.000000000	

(ii)

n							
1	0.957106781						
2	1.267228525	1.976844358	2.010462398	1.998918565	1.999796713	2.000020485	1.999999615
4	1.483036302	1.993848173	2.002974548	1.999577822	1.999980979	2.000002222	1.999999722
8	1.634748652	1.998430296	2.000776093	1.999880295	1.999998468	2.000000034	2.000000155
16	1.741802668	1.999604923	2.000196760	1.999968936	1.999999757	2.000000140	1.999999915
32	1.817445514	1.999900996	2.000049462	1.999992053	2.000000072	1.999999943	2.000000023
64	1.870919134	1.999975242	2.000012348	1.999998067	1.999999966	2.000000013	
128	1.908727207	1.999993796	2.000003116	1.999999491	2.000000005		
256	1.935460679	1.999998456	2.000000773	1.999999876			
512	1.954363881	1.999999615	2.000000193				
1024	1.967730409	1.999999904					
2048	1.977181958						

(iii)

n					
1	0.957106781				
2	1.267228525	1.976844358			
4	1.483036302	1.993848173	2.000120554		
8	1.634748652	1.998430296	2.000009838	1.999999964	
16	1.741802668	1.999604923	2.000000772	2.000000038	1.999999999
32	1.817445514	1.999900996	2.000000093	1.999999954	1.999999987
64	1.870919134	1.999975242	1.999999978	2.000000008	2.000000005
128	1.908727207	1.999993796	2.000000019	2.000000005	2.000000014
256	1.935460674	1.999998456	1.999999998	2.000000000	
512	1.954363881	1.999999615	2.000000000		
1024	1.967730409	1.999999904			
2048	1.977181958				

(iv)

n						
1	0.957106781					
2	1.267228525	1.976844358				
4	1.483036302	1.993848173	2.000044468			
8	1.634748652	1.998430296	2.000003007	1.999999950		
16	1.741802668	1.999604923	2.000000165	2.000000033	1.999999996	
32	1.817445514	1.999900996	2.000000039	1.999999899	1.999999997	
64	1.870919134	1.999975242	1.999999973	2.000000000	2.000000004	
128	1.908727207	1.999993796	2.000000189	2.000000004	2.000000002	
256	1.935460679	1.999998456	1.999999998	2.000000000		
512	1.954363881	1.999999615	2.000000000			
1024	1.967730409	1.999999964				
2048	1.977181958					

b) $-\int_0^1 x\ell nx = 0.25$

Table 3.5.2

(i)

n						
1	0.173286795					
2	0.227227184	0.245207314				
4	0.243405267	0.248797961	0.249994844			
8	0.248125746	0.249699239	0.249999665	0.249999986		
16	0.249475032	0.249924794	0.249999979	0.249999999	0.250000000	
32	0.249854656	0.249981197	0.249999998	0.249999999	0.249999999	0.250000000
64	0.249960139	0.249995300	0.250000000	0.250000001	0.250000001	0.250000001
128	0.249989153	0.249998824	0.249999999	0.249999999	0.249999999	0.249999999
356	0.249997068	0.249999706	0.250000000	0.250000000	0.250000000	0.250000000
512	0.249999212	0.249999927	0.250000000	0.250000000	0.250000000	0.250000000
1024	0.249999789	0.249999981	0.249999999	0.249999999	0.250000000	0.250000000
2048	0.249999944	0.249999996	0.250000000	0.250000000	0.250000000	0.250000000

(ii)

n							
1	0.173286795						
2	0.227227184	0.250336262	0.250045835	0.250009279	0.250002041	0.250000462	
4	0.243405267	0.250070561	0.250010133	0.250002087	0.250000465	0.250000104	
8	0.248125746	0.250015070	0.250002266	0.250000474	0.250000105	0.250000025	
16	0.249475032	0.250003279	0.250000513	0.250000107	0.250000025	0.250000006	
32	0.249854656	0.250000726	0.250000115	0.250000025	0.250000006	0.250000000	
64	0.249960139	0.250000162	0.250000027	0.250000006	0.250000001	0.250000000	
128	0.249989153	0.250000037	0.250000006	0.250000001	0.250000001		
256	0.249997068	0.250000009	0.250000001	0.250000001			
512	0.249999212	0.250000002	0.250000001				
1024	0.249999789	0.250000001					
2048	0.249999944						

(iii)

n							
1	0.173286795						
2	0.227227184	0.250336262					
4	0.243405267	0.250070561	0.250000422				
8	0.248125746	0.250015070	0.250000098	0.249999997			
16	0.249475032	0.250003279	0.250000021	0.249999994	0.249999996		
32	0.249854656	0.250000726	0.250000001	0.250000002	0.250000002	0.250000002	
64	0.249960139	0.250000162	0.250000002	0.250000001	0.250000002	0.250000002	
128	0.249989153	0.250000037	0.250000000	0.250000000	0.250000000		
256	0.249997068	0.250000009	0.249999999	0.250000000			
512	0.249999212	0.250000002	0.250000000				
1024	0.249999789	0.250000001					
2048	0.249999944						

(iv)

n							
1	0.173286795						
2	0.227227184	0.250336262					
4	0.243405267	0.250070561	0.249999676				
8	0.248125746	0.250015070	0.249999978	0.250000002			
16	0.249475032	0.250003279	0.250000000	0.249999998	0.249999999		
32	0.249854656	0.250000726	0.249999998	0.249999999	0.250000000	0.250000000	
64	0.249960139	0.250000162	0.250000002	0.250000000	0.249999999	0.250000000	
128	0.249989153	0.250000037	0.250000000	0.249999999	0.250000000		
256	0.249997068	0.250000009	0.249999999	0.249999979			
512	0.249999212	0.250000002	0.250000001				
1024	0.249999789	0.250000001					
2048	0.249999944						

c) $-\int_0^1 x\ln^3 x\,dx = 0.375.$

Table 3.5.3.

(i)

n							
1	0.083256163						
2	0.212604567	0.255720702					
4	0.299399300	0.328330878	0.352534270				
8	0.343536435	0.358248813	0.368221459	0.373450522			
16	0.362877208	0.369324132	0.373015905	0.374614054	0375001899		
32	0.370585398	0,373154795	0.374431682	0.374903608	0.375000126	0.375000007	
64	0.373460290	0.374418587	0.374839852	0.374975908	0.375000008	0.375000000	
128	0.374480996	0.374821231	0.374955446	0.374993978	0.375000001	0.375000000	
256	0.374829829	0.374946107	0.374987732	0.374998494	0.374999999	0.374999999	
512	0.374945468	0.374984014	0.374996650	0.374999623	0.375000000	0.375000000	
1024	0.374982859	0.374995323	0.374999092	0.374999906	0.375000000	0.375000000	
2048	0.374994700	0.374998647	0.374999755	0.374999976	0.375000000	0.374999999	

(ii)

n							
1	0.083256163						
2	0.212604567	0.476430459	0.358780680	0.376807956	0.375222778	0.375071265	
4	0.299399300	0.389204423	0.375291118	0.375262772	0.375072359	0.375020459	
8	0.343536435	0.377962707	0.375264567	0.375076043	0.375020751	0.375005691	
16	0.362877208	0.375693137	0.375085824	0.375021630	0.375005762	0.375001553	
32	0.370585398	0.375170303	0.375024503	0.375005978	0.375001570	0.375000419	
64	0.373460290	0.375042882	0.375006717	0.375001623	0.375000423	0.375000112	
128	0.374480996	0.375010941	0.375001810	0.375000437	0.375000113		
256	0.374829829	0.375002812	0.375000483	0.375000116			
512	0.374945468	0.375000727	0.375000128				
1024	0.374982859	0.375000188					
2048	0.374994700						

(iii)

n							
1	0.083256163						
2	0.212604567	0.476430459					
4	0.299399300	0.389204423	0.376299520				
8	0.343536435	0.377962707	0.375119032	0.375003512			
16	0.362877208	0.375693137	0.375013809	0.375000279	0.374999999		
32	0.370585398	0.375170303	0.375001820	0.375000022	0.374999999	0.375000000	
64	0.373460290	0.375042882	0.375000257	0.375000002	0.375000001	0.375000004	
128	0.374480996	0.375010941	0.375000037	0.375000001	0.375000002		
256	0.374829829	0.375002812	0.375000006	0.375000000			
512	0.374945468	0.375000727	0.375000000				
2048	0.374994700						

(iv)

n							
1	0.083256163						
2	0.212604567	0.476430459					
4	0.299399300	0.389204423	0.374133901				
8	0.343536435	0.377962707	0.374862989	0.375002432			
16	0.362887208	0.375693137	0.374975785	0.375000331	0.375000002		
32	0.370585398	0.375170303	0.374995393	0.375000050	0.375000002	0.375000002	
64	0.373460290	0.375042882	0.374999077	0.375000009	0.375000002	0.375000002	
128	0.374480996	0.375010941	0.374999808	0.375000003	0.374999985		
256	0.374829829	0.375002812	0.374999960	0.374999999			
512	0.374945468	0.375000727	0.374999990				
1024	0.374982859	0.375000188					
2048	0.374994700						

d) $-\int_0^1 x^{-\frac{1}{2}} \ln x \, dx = 4$

Table 3.5.4

(i)

n							
1	0.490129072						
2	1.021258377	2.303517949					
4	1.538191711	2.786179179	3.951426460				
8	2.006772456	3.138026446	3.987460894	3.999472372			
16	2.411783456	3.389566505	3.996837928	3.999963606	3.999996355		
32	2.750468430	3.568126288	3.999207736	3.999997672	3.999999943	4.000000000	
64	3.076986778	3.694561124	3.999801821	3.999999849	3.999999994	3.999999995	
128	3.248713040	3.784007589	3.999950457	4.000000003	4.000000013	4.000000013	
256	3.424025339	3.847266669	3.999987598	3.999999978	3.999999977	3.999999976	
512	3.561092038	3.892000322	3.999996913	4.000000018	4,000000020	4.000000021	
1024	3.667277671	3.923632467	3.999999219	3.999999998	3.999999986	3.999999985	
2048	3.748913534	3.945999942	3.999999804	3.999999999	3.999999999	4.000000000	

(ii)

n						
1	0.490129072					
2	1.021258377	20.361847506	-57.103789523	105.202365962	-86.271819968	52.403933766
4	1.538191711	6.547747802	0.397334822	7.360691847	2.095516216	4.714597290
8	2.006772456	4.992160491	3.288708487	4.435026507	3.846407146	4.047207777
16	2.411783456	4.479917916	3.811163550	4.089743653	3.985157843	4.007812787
32	2.750468430	4.256945708	3.946118791	4.026032466	4.001194268	4.003322337
64	3.026986778	4.145969174	3.986531579	4.010475344	4.002728517	4.002134194
128	3.248713040	4.086205429	3.999032048	4.005518870	4.002293818	
256	3.424025339	4.052319263	4.002502856	4.003420491		
512	3.561092038	4.032400710	4.003003510			
1024	3.667277671	4.020378974				
2048	3.748913534					

(iii)

n							
1	0.490129072						
2	1.021258377	20.361847506					
4	1.53819171	6.547747802	4.794758734				
8	2.006772456	4.992160491	4.228426300	4.036495311			
16	2.411783456	4.479917916	4.085076718	4.010457355	4.001030149		
32	2.750468430	4.256945708	4.036002505	4.003536051	4.000372926	3.999993805	
64	3.026986778	4.145969174	4.016462982	4.001365085	4.000132497	4.000033117	
128	3.248713040	4.086205429	4.007946017	4.000578875	4.000062182		
256	3.424025339	4.052319263	4.003995799	4.000267087			
512	3.561092038	4.032400710	4.002077604				
1024	3.667277671	4.020378974					
2048	3.748913544						

(iv)

n							
1	0,490129072						
2	1.021258377	20.361847506					
4	1.538191711	6.547747802	3.851136001				
8	2.006772456	4.992160491	3.965878686	4.000686057			
16	2.411783456	4.479917916	3.991907412	4.000045359	3.999998737		
32	2.750468430	4.256945708	3.998029261	4.000002130	4.000001154	4.000000001	
64	3.026986778	4.145969174	3.999512748	4.000001176	4.000002906	3.999999874	
128	3.248713040	4.086205429	3.999879277	3.999999058	3.999999940		
256	3.424025339	4.052319263	3.999969460	4.000000589			
512	3.561092038	4.032400710	3.999992591				
1024	3.667277671	4.020378974					
2048	3.748913534						

e) $-\int x^{\frac{1}{2}} \ell n x = 0.444444444...$

Table 3.5.5

(i)

n						
1	0.245064536					
2	0.358104059	0.419927427				
4	0.408090040	0.435428281	0.443905979			
8	0.429474585	0.441170181	0.444310531	0.444445381	0.444444452	
16	0.438389486	0.443265207	0.444411015	0.444444510	0.444444446	0.444444446
32	0.442030684	0.444022121	0.444436091	0.444444450	0.444444443	0.444444443
64	0.443493655	0.444293780	0.444442356	0.444444444	0.444444446	0.444444446
128	0.444073637	0.444390840	0.444443923	0.444444446	0.444444444	0.444444444
256	0.444301038	0.444425408	0.444444314	0.444444444	0.444444444	0.444444444
512	0.444389378	0.444437693	0.444444412	0.444444444	0.444444445	0.444444445
1024	0.444423429	0.444442052	0.444444436	0.444444445	0.444444445	0.444444445
2048	0.444436467	0.444443598	0.444444443	0.444444445	0.444444443	0.444444443

(ii)

n							
1	0.245064536						
2	0.358104059	0.447716653	0.444958435	0.444588932	0.444489883	0.444459234	
4	0.408090040	0.445463250	0.444615703	0.444492640	0.444459555	0.444449355	
8	0.429474585	0.444763001	0.444501025	0.444460417	0.444449455	0.444446071	
16	0.438389486	0.444544728	0.444463051	0.444449726	0.444446102	0.444444984	
32	0.442030684	0.444476236	0.444450556	0.444446188	0.444444994	0.444444624	
64	0.443493655	0.444454592	0.444446451	0.444445021	0.444444627	0.444444505	
128	0.444073637	0.444447703	0.444445105	0.444444636	0.444444506		
256	0.444301038	0.444445497	0.444444662	0.444444509			
512	0.444389378	0.444444786	0.444444462				
1024	0.444423429	0.444444557					
2048	0.444436467						

(iii)

n							
1	0.245064536						
2	0.358104059	0.447716653	0.444447290				
4	0.408090040	0.445463250	0.444447290				
8	0.429474585	0.444763001	0.444445879	0.444442831			
16	0.438389486	0.444544728	0.444444915	0.444444431	0.444444433		
32	0.442030684	0.444476236	0.444444593	0.444444433	0.444444430	0.444444433	
64	0.443493653	0.444454592	0.444444486	0.444444448	0.444444445	0.444444446	
128	0.444073637	0.444447703	0.444444458	0.444444444	0.444444446		
256	0.444301038	0.444445497	0.444444449	0.444444447			
512	0.444389378	0.444444786	0.444444447				
1024	0.444423429	0.444444557					
2048	0.444436467						

(iv)

n							
1	0.245064536						
2	0.358104059	0.447716653					
4	0.408090040	0.445463250	0.444418900				
8	0.429474585	0.44476300k	0.444439162	0.444444398			
16	0.438389486	0.444544728	0.444443270	0.444444449	0.444444440		
32	0.442030684	0.444476236	0.444444178	0.444444438	0.444444443	0.444444446	
64	0.443493653	0.444454592	0.444444379	0.444444448	0.444444445	0.444444447	
128	0.444073637	0.444447703	0.444444430	0.444444444	0.444444446		
256	0.444301038	0.444445497	0.444444441	0.444444447			
512	0.444389378	0.444444786	0.444444445				
1024	9.444423429	0.444444557					
2048	0.444436467						

3.7 CONCLUSION

Numerical quadrature for endpoint singularity integrands and linear and non-linear extrapolation processes have been briefly surveyed. Using a geometrical approach, the extrapolation processes were considered as finding the solution to a fixed-point problem. The Aitken processes and the ε-algorithm give accelerated values $x_{j,k}$ $(k = 2,3...)$ of the converging sequences $\{x_{j,1}\}$ $(\{x_j\})$ with errors of order k. The asymptotic error constant $a_{k,k}$ of these error terms involve the factor $(a_1)^k$ so the rates of convergence mostly depend on the size of a_1. The approach here is similar to the idea suggested by Johnson [8].

There are some other extrapolation processes [9] which have not been mentioned here. Different processes have different approaches and algorithms. However, Brezinski [1] give a general formalism for these linear and non-linear extrapolation processes. This formalism includes most of the sequence transformations actually used for convergence acceleration. It also includes rational extrapolation. It will be discussed in the next chapter.

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CHAPTER 4

A GENERAL ALGORITHM FOR RATIONAL INTERPOLATION

4.1 INTRODUCTION

Recently Brezinski [1] presented a very effective general extrapolation algorithm for linear and rational extrapolation. This algorithm was extended by Brezinski to a general interpolation algorithm which is called the Muhlbach-Neville-Aitken (MNA) Algorithm in [2]. In this chapter, the rational interpolating function is generalized in a similar way. This method answers the question raised in [2] by Brezinski. The aim of this chapter is to present an algorithm for recursively constructing the interpolating rational function.

$$R^{i}_{m,n}(x) = \frac{\sum_{j=0}^{m} a_j\, h_j(x)}{\sum_{j=0}^{n} b_j\, h_j(x)} \qquad (4.1.1)$$

With $R^{i}_{m,n}(x_j) = f_j$, $j = i, i+1 \ldots i+m+n$, $i=0,1,2\ldots$, from either $R^{i}_{m,n-1}(x)$ or $R^{i}_{m-1,n}(x)$ by an extension of the MNA algorithm. The set of given functions $[\{h_j(x)\}_{j=0}^{m}, \{h_j(x)f(x)\}_{j=1}^{n}]$ is assumed to form a complete or quasicomplete Chebyshev system [8] on the set of interpolating points.

Instead of setting $R^{i}_{n,0}(x) = \dfrac{1}{R^{i}_{0,n}(x)}$ $\quad n = 1,2 \ldots$

for the rational function (as in [2]), This algorithm is applied to the rational fraction $R^{i}_{0,n}(x)$ directly. Then the $R^{i}_{m,n}(x)$ can be generated either from the (m-1)th row vertically or from the (n-1)th column horizontally. If (N+1) interpolating points are given, the following triangular array of the interpolating function can be constructed.

$$
\begin{array}{llll}
R^{i}_{0,0} & R^{i}_{0,1} \cdots & R^{i}_{0,n-1} & R^{i}_{0,n} \\
R^{i}_{1,0} & R^{i}_{1,1} \cdots & R^{i}_{1,n-1} & \\
\vdots & \vdots & & \\
R^{i}_{n-1,0} & R^{i}_{n-1,1} & & \\
R^{i}_{n,0} & & &
\end{array}
$$

Figure 4.1.1

In this array, each term $R^{i}_{m,n}$ represents a table of functions for $i = 0,1\ldots, N-m-n$.

This algorithm is more general than the algorithms suggested by Larkin [6]. With the normalization $b_0 = 1$, $R^{i}_{m,n}(x)$ is expressed implicitly in the form

$$h_0(x)R^{i}_{m,n}(x) = R^{i}_{m,n}(x) \sum_{j=1}^{n} b_j h_j(x) + \sum_{j=0}^{m} a_j h_j(x) \qquad (4.1.2)$$

By using this algorithm, the coefficients of the interpolating function can be determined easily. The interpolating value at a given point x=a can be found implicitly. However for computational convenience, the representation can be transformed to a new basis, $\bar{h}_j(x) = h_j(x) - h_j(a)$ $\forall j > 0$, so that $\bar{h}_j(a) = 0$, $\forall j > 0$. In this case interpolation will be reduced to general rational extrapolation.

In Section 4.2 the MNA algorithm [2] is reviewed. The extension of this algorithm to generalized rational functions is given in Section 4.3. In Section 4.4 there is a discussion on how to overcome the problem when the algorithm breaks down due to a zero divisor. Some examples and numerical results are given in Section 4.5.

4.2 THE MNA ALGORITHM

The MNA algorithm [2] is reviewed.

Suppose the polynomials are considered

$$P_k^n(x) = a_0 g_0(x) + \dots + a_k g_k(x) \quad ,$$

$$\text{such that } P_k^n(x_i) = f_i \ ,$$

where (x_i, f_i) $i = n \dots n+k$ are the interpolating points.

Then $P_k^n(x)$ can be expressed as

$$P_k^n(x) = \frac{\begin{vmatrix} 0 & -f_n & \dots & -f_{n+k} \\ g_0(x) & g_0(x_n) & \dots & g_0(x_{n+k}) \\ \dots & \dots & \dots & \dots \\ g_k(x) & g_k(x_n) & \dots & g_k(x_{n+k}) \end{vmatrix}}{D} \qquad (4.2.1)$$

Note: In this chapter D is the minor obtained by eliminating the first row and the first column of the determinant.

Now let $g_{k,i}^n(x)$ be the ratio of determinants obtained by replacing the first row in the numerator of P_k^n by

$$(-g_i(x) \quad -g_i(x_n) \quad \dots \quad -g_i(x_{n+k}))$$

Note that $g^n_{k,i}(x) = 0$, $i \leqslant k$ and $g^n_{k,i}(x_j) = 0$, $j = n \ldots n+k$.

Then the MNA algorithm is the following :

$$P^n_0(x) = \frac{\begin{vmatrix} 0 & -f_n \\ g_0(x) & g_0(x_n) \end{vmatrix}}{g_0(x_n)} = f_n \frac{g_0(x)}{g_0(x_n)} ,$$

$$g^n_{0,i}(x) = \frac{\begin{vmatrix} -g_i(x) & -g_i(x_n) \\ g_0(x) & g_0(x_n) \end{vmatrix}}{g_0(x_n)} = g_i(x_n)\frac{g_0(x)}{g_0(x_n)} - g_i(x), \quad i = 1,2 \ldots$$

For $k = 1,2 \ldots$ and $n = 0,1 \ldots$

$$P^n_k(x) = \frac{g^{n+1}_{k-1,k}(x)\, P^n_{k-1}(x) - g^n_{k-1,k}(x)\, P^{n+1}_{k-1}(x)}{g^{n+1}_{k-1,k}(x) - g^n_{k-1,k}(x)}$$

$$= P^n_{k-1}(x) - \frac{\Delta P^n_{k-1}(x)}{\Delta g^n_{k-1}(x)} g^n_{k-1,k}(x) \qquad (4.2.2a)$$

$$g^n_{k,i}(x) = \frac{g^{n+1}_{k-1,k}(x)\, g^n_{k-1,i}(x) - g^n_{k-1,k}(x)\, g^{n+1}_{k-1,i}(x)}{g^{n+1}_{k-1,k}(x) - g^n_{k-1,k}(x)}$$

$$= g^n_{k-1,i}(x) - \frac{\Delta g^n_{k-1,i}(x)}{\Delta g^n_{k-1,k}(x)} g^n_{k-1,k}(x) \quad i = k+1, k+2 \ldots \qquad (4.2.2b)$$

and Δ is the forward difference on the index n.

The way of computing $g^n_{k,i}(x)$ in [2] is equivalent to Aitken's pattern. With the initialization of $g^n_{0,i}(x)$ for a fixed value of n, it can be shown in Figure 4.2.1

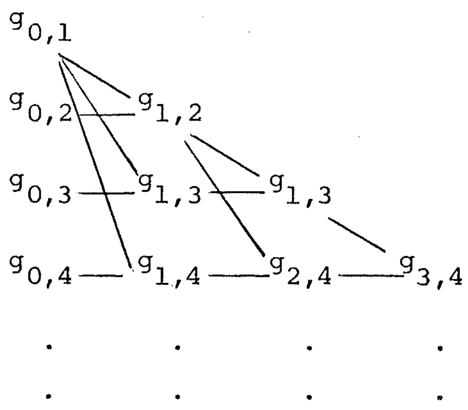

Figure 4.2.1

To show the relationship to its generalization, this algorithm is essentially restated in a new notation.

For convenience, instead of using $g^n_{k,i}(x)$, initialize

$$Vg^{\,n}_{1-k,k}(x) = Hg^{\,n}_{1-k,k}(x) = \frac{\begin{vmatrix} -g_k(x) & -g_k(x_n) \\ g_0(x) & g_0(x_n) \end{vmatrix}}{g_0(x_n)} \tag{4.2.3a}$$

$$k = 1,2 \;\ldots.$$

Note: $Vg^n_{k,0}(x)$ is used to generate $P^n_k(x)$ vertically.

$Hg^n_{0,k}(x)$ is used to generate $P^n_k(x)$ horizontally.

Define $Hg^{\,n}_{-j,k}(x) = 0$ and $Vg^{\,n}_{-j,k}(x) = 0$ when $j \geqslant k$.

For $i = 2,3,4 \ldots$, $j = 0,1,2 \ldots$, and $k = j+i$.

$$Hg^{\,n}_{-j,k}(x) = \frac{Hg^{\,n}_{-(j+1),k}(x)\; Vg^{\,n+1}_{-j,k-1}(x) - Hg^{\,n+1}_{-(j+1),k}(x)\; Vg^{\,n}_{-j,k-1}(x)}{Vg^{\,n+1}_{-j,k-1}(x) - Vg^{\,n}_{-j,k-1}(x)}$$

$$= Hg^{\,n}_{-(j+1),k}(x) - \frac{\Delta\, Hg^{\,n}_{-(j+1),k}(x)}{\Delta\, Vg^{\,n}_{-j,k-1}(x)}\; Vg^{\,n}_{-j,k-1}(x) \tag{4.2.3b}$$

$$Vg^{\,n}_{-j,k}(x) = \frac{Vg^{\,n}_{-j,k-1}(x)\ Hg^{\,n+1}_{-(j+1),k}(x) - Vg^{\,n+1}_{-j,k-1}(x)\ Hg^{\,n}_{-(j+1),k}(x)}{Hg^{\,n+1}_{-(j+1),k}(x) - Hg^{\,n}_{-(j+1),k}(x)}$$

$$= Vg^{\,n}_{-j,k-1}(x) - \frac{\Delta\, Vg^{\,n}_{-j,k-1}(x)}{\Delta\, Hg^{\,n}_{-(j+1),k}(x)}\, Hg^{\,n}_{-(j+1),k}(x) \qquad (4.2.3c)$$

$$\text{where } Hg^{\,n}_{-j,k}(x) = \frac{\begin{vmatrix} -g_k(x) & -g_k(x_n) & \cdots & -g_k(x_{n+k-j-1}) \\ g_0(x) & g_0(x_n) & \cdots & g_0(x_{n+k-j-1}) \\ g_{j+1}(x) & g_{j+1}(x_n) & \cdots & g_{j+1}(x_{n+k-j-1}) \\ \cdots & \cdots & \cdots & \cdots \\ g_{k-1}(x) & g_{k-1}(x_n) & \cdots & g_{k-1}(x_{n+k-j-1}) \end{vmatrix}}{\begin{vmatrix} g_0(x_n) & \cdots & g_0(x_{n+k-j-1}) \\ g_{j+1}(x_n) & \cdots & g_{j+1}(x_{n+k-j-1}) \\ \cdots & \cdots & \cdots \\ g_{k-1}(x_n) & \cdots & g_{k-1}(x_{n+k-j-1}) \end{vmatrix}} \qquad (4.2.3d)$$

$$Vg^{\,n}_{-j,k}(x) = \frac{\begin{vmatrix} -g_k(x) & -g_k(x_n) & \cdots & -g_k(x_{n+k-j-1}) \\ g_0(x) & g_0(x_n) & \cdots & g_0(x_{n+k-j-1}) \\ g_{j+1}(x) & g_{j+1}(x_n) & \cdots & g_{j+1}(x_{n+k-j-1}) \\ \cdots & \cdots & \cdots & \cdots \\ g_{k-1}(x) & g_{k-1}(x_n) & \cdots & g_{k-1}(x_{n+k-j-1}) \end{vmatrix}}{\begin{vmatrix} g_0(x_n) & \cdots & g_0(x_{n+k-j-1}) \\ g_{j+2}(x_n) & \cdots & g_{j+2}(x_{n+k-j-1}) \\ \cdots & \cdots & \cdots \\ g_k(x_n) & \cdots & g_k(x_{n+k-j-1}) \end{vmatrix}} \qquad (4.2.3e)$$

$$\text{and } Hg^{\,n}_{0,k}(x) = \frac{\begin{vmatrix} -g_k(x) & -g_k(x_n) & \cdots & -g_0(x_{n+k-j-1}) \\ g_0(x) & g_0(x_n) & \cdots & g_0(x_{n+k-j-1}) \\ \cdots & \cdots & \cdots & \cdots \\ g_{k-1}(x) & g_{k-1}(x_n) & \cdots & g_{k-1}(x_{n+k-j-1}) \end{vmatrix}}{D} \qquad (4.2.3f)$$

This is equivalent to Neville pattern and the way of computing can be shown by Figure 4.2.2.

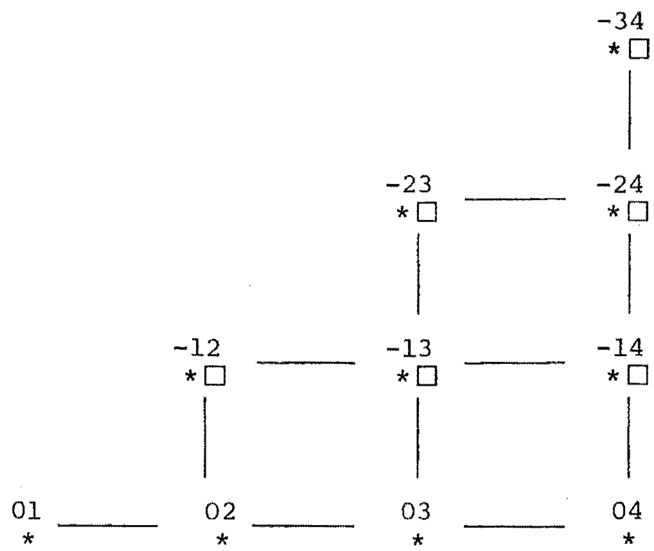

Figure 4.2.2 * Hg □ Vg

Then $$P_k^n(x) = P_{k-1}^n(x) - \frac{\Delta P_{k-1}^n(x)}{\Delta Hg_{0,k}^n(x)} Hg_{0,k}^n(x) \qquad (4.2.3g)$$

$k = 1,2....$

Alternatively, if it is initialized

$$Vg^n_{k,1-k}(x) = \frac{\begin{vmatrix} -g_k(x) & -g_k(x_n) \\ g_0(x) & g_0(x_n) \end{vmatrix}}{g_0(x_n)}$$

$$Hg^n_{k,1-k}(x) = \frac{\begin{vmatrix} -g_k(x) & -g_k(x_n) \\ g_0(x) & g_0(x_n) \end{vmatrix}}{g_0(x_n)} \qquad (4.2.3h)$$

$k = 1,2,3....$

then by using(4.2,3c,d) to compute $Hg^n_{k,-j}(x)$ and $Vg^n_{k,-j}(x)$ it can be shown

$$P^n_k(x) = P^n_{k-1} - \frac{\Delta\, P^n_{k-1}(x)}{\Delta\, Vg^n_{k,0}(x)}\, Vg^n_{k,0}(x) \qquad (4.2.3i)$$

and $Vg^n_{k,0}(x)$ has the same form as(4.2.3f).

For linear interpolation, it is better to use the Aitken pattern rather than the Neville since it uses less storage and computation. But for the rational interpolation, Neville pattern is more effective and economical. The ratios of the differences in(4.2.2) and (4.2.3b,c) are constant terms as shown in the following lemma.

LEMMA 1:

The ratio of the differences in (4.2.3b) *and* (4.2.3c) *are constants* (*independent of* x).

Proof:

With the definition of $Hg^n_{-(j+1),k}(x)$ and $Hg^n_{-j,k-1}(x)$ in (4.2.3d,e) by using the Sylvester's identity and exchanging some rows or columns in (4.2.3b), after term eliminating, then

$$\frac{\Delta\, Hg^{\,n}_{-(j+1),k}(x)}{\Delta\, Vg^{\,n}_{-j,k-1}(x)} =$$

$$\left\{ - \begin{vmatrix} g_0(x_n) & g_0(x) & g_0(x_{n+1}) & \cdot & g_0(x_{n+k-j-1}) \\ g_{j+2}(x_n) & g_{j+2}(x) & g_{j+2}(x_{n+1}) & \cdot & g_{j+2}(x_{n+k-j-1}) \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ g_{k-1}(x_n) & g_{k-1}(x) & g_{k-1}(x_{n+1}) & \cdot & g_{k-1}(x_{n+k-j-1}) \\ 0 & 1 & 0 & \cdots & 0 \end{vmatrix} \begin{vmatrix} -g_k(x) & -g_k(x_{n+1}) & \cdots & -g_k(x_{n+k-j}) \\ g_0(x) & g_0(x_{n+1}) & \cdots & g_0(x_{n+k-j}) \\ g_{j+2}(x) & g_{j+2}(x_{n+1}) & \cdots & g_{j+2}(x_{n+k-j}) \\ \cdots & \cdots & \cdots & \cdots \\ g_{k-1}(x) & g_{k-1}(x_{n+1}) & \cdots & g_{k-1}(x_{n+k-j}) \end{vmatrix} + \right.$$

$$\left. \begin{vmatrix} g_0(x) & g_0(x_{n+1}) & \cdots & g_0(x_{n+k-j}) \\ g_{j+2}(x) & g_{j+2}(x_{n+1}) & \cdots & g_{j+2}(x_{n+k-j}) \\ \cdots & \cdots & \cdots & \cdots \\ g_{k-1}(x) & g_{k-1}(x_{n+1}) & \cdots & g_{k-1}(x_{n+k-j}) \\ 1 & 0 & \cdots & 0 \end{vmatrix} \begin{vmatrix} -g_k(x_n) & -g_k(x) & -g_k(x_{n+1}) & \cdots & -g_k(x_{n+k-j-1}) \\ g_0(x_n) & g_0(x) & g_0(x_{n+1}) & \cdots & g_0(x_{n+k-j-1}) \\ g_{j+2}(x_n) & g_{j+2}(x) & g_{j+2}(x_{n+1}) & \cdot & g_{j+2}(x_{n+k-j-1}) \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ g_{k-1}(x_n) & g_{k-1}(x) & g_{k-1}(x_{n+1}) & \cdot & g_{k-1}(x_{n+k-j-1}) \end{vmatrix} \right\} \Big/$$

$$\left\{ - \begin{vmatrix} g_0(x_n) & g_0(x) & g_0(x_{n+1}) & \cdots & g_0(x_{n+k-j-1}) \\ g_{j+2}(x_0) & g_{j+2}(x) & g_{j+2}(x_{n+1}) & \cdot & g_{j+2}(x_{n+k-j-1}) \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ g_{k-1}(x_n) & g_{k-1}(x) & g_{k-1}(x_{n+1}) & \cdot & g_{k-1}(x_{n+k-j-1}) \\ 0 & 1 & 0 & \cdots & 0 \end{vmatrix} \begin{vmatrix} -g_{k-1}(x) & -g_{k-1}(x_{n+1}) & \cdots & -g_{k-1}(x_{n+k-j}) \\ g_0(x) & g_0(x_{n+1}) & \cdots & g_0(x-1+k-j) \\ g_{j+1}(x) & g_{j+1}(x_{n+1}) & \cdots & g_{j+1}(x_{n+k-j}) \\ \cdots & \cdots & \cdots & \cdots \\ g_{k-2}(x) & g_{k-2}(x_{n+1}) & \cdots & g_{k-2}(x_{n+k-j}) \end{vmatrix} + \right.$$

$$\left. \begin{vmatrix} g_0(x) & g_0(x_{n+1}) & \cdots & g_0(x_{n+k-j}) \\ g_{j+2}(x) & g_{k+2}(x_{n+1}) & \cdots & g_{k+2}(x_{n+k-j}) \\ \cdots & \cdots & \cdots & \cdots \\ g_{k-1}(x) & g_{k-1}(x_{n+1}) & \cdots & g_{k-1}(x_{n+k-j}) \\ 1 & 0 & \cdots & 0 \end{vmatrix} \begin{vmatrix} -g_{k-1}(x_n) & -g_{k-1}(x) & -g_{k-1}(x_{n+1}) & \cdot & g_{k-i}(x_{n+k-j-1}) \\ g_0(x_n) & g_0(x) & g_0(x_{n+1}) & \cdots & g_0(x_{n+k-j-1}) \\ g_{j+1}(x_n) & g_{j+1}(x) & g_{j+1}(x_{n+1}) & \cdot & g_{j+1}(x_{n+k-j-1}) \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ g_{k-2}(x_n) & g_{k-2}(x) & g_{k-2}(x_{n+1}) & \cdot & g_{k-2}(x_{n+k-j-1}) \end{vmatrix} \right\}$$

$$
= (-1)^{k-j} \frac{\begin{vmatrix} -g_k(x) & -g_k(x_n) & \cdots & -g_k(x_{n+k-j}) \\ g_0(x) & g_0(x_n) & \cdots & g_0(x_{n+k-j}) \\ g_{j+2}(x) & g_{j+2}(x_n) & \cdots & g_{j+2}(x_{n+k-j}) \\ \cdots & \cdots & \cdots & \cdots \\ g_{k-1}(x) & g_{k-1}(x_n) & \cdots & g_{k-1}(x_{n+k-j}) \\ 1 & 0 & \cdots & 0 \end{vmatrix}}{\begin{vmatrix} g_{j+1}(x) & g_{j+1}(x_n) & \cdots & g_{j+1}(x_{n+k-j}) \\ g_0(x) & g_0(x_n) & \cdots & g_0(x_{n+k-j}) \\ g_{j+2}(x) & g_{j+2}(x_n) & \cdots & g_{j+2}(x_{n+k-j}) \\ \cdots & \cdots & \cdots & \cdots \\ -g_{k-1}(x) & -g_{k-1}(x_n) & \cdots & -g_{k-1}(x_{n+k-j}) \\ 1 & 0 & \cdots & 0 \end{vmatrix}} = \frac{\begin{vmatrix} -g_k(x_n) & \cdots & -g_k(x_{n+k-j}) \\ g_0(x_n) & \cdots & g_0(x_{n+k-j}) \\ g_{j+2}(x_n) & \cdots & g_{j+2}(x_{n+k-j}) \\ \cdots & \cdots & \cdots \\ g_{k-1}(x_n) & \cdots & g_{k-1}(x_{n+k-j}) \end{vmatrix}}{\begin{vmatrix} -g_{k-1}(x_n) & \cdots & g_{k-1}(x_{n+k-j}) \\ g_0(x_n) & \cdots & g_0(x_{n+k-j}) \\ g_{j+1}(x_n) & \cdots & g_{j+1}(x_{n+k-j}) \\ \cdots & \cdots & \cdots \\ g_{k-2}(x_n) & \cdots & g_{k-2}(x_{n+k-j}) \end{vmatrix}} = \textit{constant}
$$

where $j + 2 < k$

(4.2.3c) can be proved similarly.

LEMMA 2:

The ratios of the differences in (4.2.3g) *and* (4.2.3i) *are constants*

Proof: Similar to Lemma 1.

It is interesting to observe that $g^n_{k-1,k}(x)\,[\nabla g^n_{k,0}(x)\ \ Hg^n_{0,k}(x)]$ in the algorithm acts to increase the degree of $P^n_k(x)$. The key of this algorithm is to build up $g^n_{k,i}(x)[\nabla g^n_{k,i}(x)\ \ Hg^n_{k,i}(x)]$ These play an important role in the generalization to the rational interpolating function $R^i_{m,n}(x)$ with $R^i_{m,n}(x_j) = f_j$ where $j = i, i+1 \ldots i+m+n$.

4.3 THE RATIONAL INTERPOLATION ALGORITHM

The interpolating rational function $R^i_{m,n}(x)$(4.1.1) may be expressed implicitly in the form (4.1.2). Then $h_0(x)R^i_{m,n}(x)$ can be expressed in the same form as(4.2.1) where f_j is replaced by $h_0(x_j)f_j$, $j = i, i+1, \ldots, i+m+n$ and $g_k(x) = h_k(x)$, $k = 0,1,\ldots,m$; $g_{m+\ell}(x) = h_\ell(x)R^i_{m,n}(x)$, $\ell = 1,2,\ldots,n$.

If it is assumed $g_k(x) = x^k$, $k = 0,1,2,\ldots m$, $g_{m+\ell}(x) = x^\ell f(x)$ $\ell = 1,2\ldots n$, then $R^i_{m,n}(x)$ can be expressed as below (4.3.1)

(Clearly a minor notational change will suffice to handle the more general case when $h_0(x)$ is not identically 1).

$$R^i_{m,n}(x) = \frac{\begin{vmatrix} 0 & -f_i & \cdots & -f_{i+m+n} \\ 1 & 1 & \cdots & 1 \\ x & x_i & \cdots & x_{i+m+n} \\ \cdots & \cdots & \cdots & \cdots \\ x^m & x_i^m & \cdots & x_{i+m+n}^m \\ xf & x_if_i & \cdots & x_{i+m+n}f_{i+m+n} \\ \cdots & \cdots & \cdots & \cdots \\ x^nf & x_i^nf_i & \cdots & x_{i+m+n}^nf_{i+m+n} \end{vmatrix}}{D} \tag{4.3.1}$$

$g^i_{m-1,m}(x)$ can be built up where $m = 1,2\ldots$ for computing $R^i_{m,0}(x)$, and $g^i_{n-1,n}(x)$ where $n = 1,2\ldots$ for computing $R^i_{0,n}(x)$ by using(4.2.2) which is based on Aitken's pattern, or built up $Vg^i_{m,0}(x)$ for $R^i_{m,0}(x)$ and $Hg^i_{0,n}(x)$for $R^i_{0,n}(x)$by using(4.2.3) which is based on Neville pattern. Then by using the relation of $Vg^i_{m,0}(x)$ $(g^i_{m-1,m}(x))$ and $Hg^i_{0,n}(x)$ $(g^i_{n-1,n}(x))$ it is possible to build up

$Vg^{i}_{m,n}(x)$ and $Hg^{i}_{m,n}(x)$ which is based on Neville's pattern for constructing $R^{i}_{m,n}(x)$ either from the previous column or row. The following algorithm is based on the Neville pattern.

1. Initialization.

For m,n = 1,2,... N and for i = 0,1,...,N-1

$$Vg^{i}_{m,1-m}(x) = \frac{\begin{vmatrix} -g_m(x) & -g_m(x_i) \\ g_0(x) & g_0(x_i) \end{vmatrix}}{g_0(x_i)}.$$

$$Hg^{i}_{m,1-m}(x) = \frac{\begin{vmatrix} -g_m(x) & -g_m(x_i) \\ g_0(x) & g_0(x_i) \end{vmatrix}}{g_0(x_i)} \qquad (4.3.2a)$$

where $g_0(x_i) = 1$ $\qquad$ m = 1,2 ....

$g_m(x_i) = x_i^m$ $\qquad$ i = 0,1 ....

$$Vg^{i}_{1-n,n}(x) = \frac{\begin{vmatrix} -g_n(x) & -g_n(x_i) \\ g_0(x) & g_0(x_i) \end{vmatrix}}{g_0(x_i)}$$

$$Hg^{i}_{1-n,n}(x) = \frac{\begin{vmatrix} -g_n(x) & -g_n(x_i) \\ g_0(x) & g_0(x_i) \end{vmatrix}}{g_0(x_i)} \qquad (4.3.2b)$$

where $g_n(x_i) = x_i^n f_i$

$g_0(x_i) = 1$ $\qquad$ n = 1,2 ...

2. For $k = 2,3,\ldots,N$

For $m = N, N-1,\ldots,k-N$

Set $n = k - m$

For $i = 0,1,\ldots,N-k$

$$Hg^i_{m,n}(x) = Hg^i_{m-1,n}(x) - \frac{\Delta\, Hg^i_{m-1,n}(x)}{\Delta\, Vg^i_{m,n-1}(x)}\, Vg^i_{m,n-1}(x) \tag{4.3.2c}$$

$$Vg^i_{m,n}(x) = Vg^i_{m,n-1}(x) - \frac{\Delta\, Vg^i_{m,n-1}(x)}{\Delta\, Hg^i_{m-1,n}(x)}\, Hg^i_{m-1,n}(x) \tag{4.3.2d}$$

3. For $i = 0, 1,\ldots,N$, define $R^i_{0,0}(x) = f_i$

For $n = 1,2,\ldots,N$

For $i = 0,1,\ldots,N-n$

$$R^i_{0,n}(x) = R^i_{0,n-1}(x) - \frac{\Delta\, R^i_{0,n-1}(x)}{\Delta\, Hg^i_{0,n}(x)}\, Hg^i_{0,n}(x) .$$

For $m = 1,2,\ldots,N$

For $i = 0,1,\ldots,N-m$

$$R^i_{m,0}(x) = R^i_{m-1,0}(x) - \frac{\Delta\, R^i_{m-1,0}(x)}{\Delta\, Vg^i_{m,0}(x)}\, Vg^i_{m,0}(x)$$

For $m,n = 1,2,\ldots N$

For $i = 0,1,\ldots,N-m-n$

$$R^i_{m,n}(x) = R^i_{m,n-1}(x) - \frac{\Delta\, R^i_{m,n-1}(x)}{\Delta\, Hg^i_{m,n}(x)}\, Hg^i_{m,n}(x) \tag{4.3.2e}$$

$$R^i_{m,n}(x) = R^i_{m-1,n}(x) - \frac{\Delta\, R^i_{m-1,n}(x)}{\Delta\, Vg^i_{m,n}(x)}\, Vg^i_{m,n}(x) \tag{4.3.2f}$$

The algorithm follows from the relations proved in the following Theorem.

<u>THEOREM 1</u>

Equations (4.3.2e) *and* (4.3.2f) *hold for* $m,n = 0,1,2\ldots\ldots$ *provided* $n > 1$ *for* (4.3.2e) *and* $m > 1$ *for* (4.3.2f).

Proof: To prove (4.3.2e) use the Sylvester's identity for the determinants, $R^i_{m,n}(x)$ can be decomposed as the following:

$$R^i_{m,n}(x) = \frac{\begin{vmatrix} 0 & -f_i & \cdots & -f_{i+m+n-1} \\ 1 & 1 & \cdots & 1 \\ x & x_i & \cdots & x_{i+m+n-1} \\ \cdots & \cdots & \cdots & \cdots \\ x^m & x_i^m & \cdots & x^m_{i+m+n-1} \\ xf & x_i f_i & \cdots & x_{i+m+n-1}\, f_{i+m+n-1} \\ \cdots & \cdots & \cdots & \cdots \\ x^{n-1}f & x_i^{n-1} f_i & \cdots & x_{i+m+n-1}\, f_{i+m+n-1} \end{vmatrix}}{D} -$$

$$\frac{\begin{vmatrix} -f_i & \cdots & -f_{i+m+n} \\ 1 & \cdots & 1 \\ x_i & \cdots & x_{i+m+n} \\ \cdots & \cdots & \cdots \\ x_i^m & \cdots & x^m_{i+m+n} \\ x_i f_i & \cdots & x_{i+m+n} f_{i+m+n} \\ \cdots & \cdots & \cdots \\ x_i^{n-1} f_i & \cdots & x^{n-1}_{i+m+n} f_{i+m+n} \end{vmatrix} \cdot \begin{vmatrix} 1 & & \cdots & 1 \\ x & x_i & \cdots & x_{i+m+n-1} \\ \cdots & & \cdots & \cdots \\ x^m & x_i^m & \cdots & x^m_{i+m+n-1} \\ xf & x_i f_i & \cdots & x_{i+m+n-1} f_{i+m+n-1} \\ \cdots & & \cdots & \cdots \\ x^n f & x_i^n f_i & \cdots & x^n_{i+m+n-1} f_{i+m+n-1} \end{vmatrix}}{\begin{vmatrix} 1 & \cdots & 1 \\ x_i & \cdots & x_{i+m+n} \\ \cdots & \cdots & \cdots \\ x_i^m & \cdots & x^m_{i+m+n} \\ x_i f_i & \cdots & x_{i+m+n} f_{i+m+n} \\ \cdots & \cdots & \cdots \\ x_i^n f_i & \cdots & x^n_{i+m+n} f_{i+m+n} \end{vmatrix} \cdot \begin{vmatrix} 1 & \cdots & 1 \\ x_i & \cdots & x_{i+m+n-1} \\ \cdots & \cdots & \cdots \\ x_i^m & \cdots & x^m_{i+m+n-1} \\ x_i f_i & \cdots & x_{i+m+n-1} f_{i+m+n-1} \\ \cdots & \cdots & \cdots \\ x_i^{n-1} f_i & \cdots & x^{n-1}_{i+m+n-1} f_{i+m+n-1} \end{vmatrix}}$$

Define

$$Hg^{i}_{m,n}(x) = \frac{\begin{vmatrix} -x^n f & -x_i^n f_i & \cdots & -x^n_{i+m+n-1} f_{i+m+n-1} \\ 1 & 1 & \cdots & 1 \\ x & x_i & \cdots & x_{i+m+n-1} \\ \cdots & \cdots & \cdots & \cdots \\ x^m & x_i^m & \cdots & x^m_{i+m+n-1} \\ xf & x_i f_i & \cdots & x_{i+m+n-1} f_{i+m+n-1} \\ \cdots & \cdots & \cdots & \cdots \\ x^{n-1} f & x_i^{n-1} f_i & \cdots & x^{n-1}_{i+m+n-1} f_{i+m+n-1} \end{vmatrix}}{\begin{vmatrix} 1 & \cdots & 1 \\ x_i & \cdots & x_{i+m+n-1} \\ \cdots & \cdots & \cdots \\ x_i^m & \cdots & x^m_{i+m+n-1} \\ x_i f_i & \cdots & x_{i+m+n-1} f_{i+m+n-1} \\ \cdots & \cdots & \cdots \\ x_i^{n-1} f_i & \cdots & x^{n-1}_{i+m+n-1} f_{i+m+n-1} \end{vmatrix}} \qquad (4.3.2g)$$

which is the second factor of the second term by shifting the last row to the first row and change the sign. The first factor of the second term is in fact equal to $\dfrac{\Delta\, R^{i}_{m,n-1}(x)}{\Delta\, Hg^{i}_{m,n}(x)}$.

In the same way as in lemma 1, it can be shown that

$$\frac{\Delta\, R^{i}_{m,n-1}(x)}{\Delta\, Hg^{i}_{m,n}(x)} = \frac{\begin{vmatrix} -f_i & \cdots & -f_{i+m+n} \\ 1 & \cdots & 1 \\ x_i & \cdots & x_{i+m+n} \\ \cdots & \cdots & \cdots \\ x_i^m & \cdots & x_{i+m+n}^m \\ x_i f_i & \cdots & x_{i+m+n} f_{i+m+n} \\ \cdots & \cdots & \cdots \\ x_i^{n-1} f_i & \cdots & x_{i+m+n}^{n-1} f_{i+m+n} \end{vmatrix}}{\begin{vmatrix} -x_i^n f_i & \cdots & -x_{i+m+n}^{n-1} f_{i+m+n} \\ 1 & \cdots & 1 \\ x_i & \cdots & x_{i+m+n} \\ \cdots & \cdots & \cdots \\ x_i^m & \cdots & x_{i+m+n}^m \\ x_i f_i & \cdots & x_{i+m+n} f_{i+m+n} \\ \cdots & \cdots & \cdots \\ x_i^n f_i & \cdots & x_{i+m+n}^{n-1} f_{i+m+n} \end{vmatrix}}$$

which is a constant formed by the interpolating set $\{(x_j, f_j),\ j = i, \ldots\ i+m+n\}$

To prove (4.3.2f), shift the mth row of the numerator in (4.3.1) to the last row and the proof follows using the same method as above, where in this case the second factor is defined to be $Vg^{i}_{m,n}(x)$

that is

$$Vg^{i}_{m,n}(x) = \frac{\begin{vmatrix} -x^n f & -x_i^n f_i & \cdots & -x^n_{i+m+n-1} f_{i+m+n-1} \\ 1 & 1 & \cdots & 1 \\ x & x_i & \cdots & x_{i+m+n-1} \\ \cdots & \cdots & \cdots & \cdots \\ x^m & x_i^m & \cdots & x^m_{i+m+n-1} \\ xf & x_i f_i & \cdots & x_{i+m+n-1} f_{i+m+n-1} \\ \cdots & \cdots & \cdots & \cdots \\ x^{n-1} f & x_i^{n-1} f_i & \cdots & x^{n-1}_{i+m+n-1} f_{i+m+n-1} \end{vmatrix}}{\begin{vmatrix} 1 & \cdots & 1 \\ x_i & \cdots & x_{i+m+n-1} \\ \cdots & \cdots & \cdots \\ x_i^{m-1} & \cdots & x^{m-1}_{i+m+n-1} \\ x_i f_i & \cdots & x_{i+m+n-1} f_{i+m+n-1} \\ \cdots & \cdots & \cdots \\ x_i^n f_i & \cdots & x^n_{i+m+n-1} f_{i+m+n-1} \end{vmatrix}} \qquad (4.3.2h)$$

Note: 1. The expressions for $Hg^{i}_{m,n}(x)$ and $Vg^{i}_{m,n}(x)$ have common numerators and the denominators have one row different.

2. The expressions for $Hg^{i}_{m-1,n}(x)$ and $Vg^{i}_{m,n-1}(x)$ have the same denominators but the numerators have one row different.

THEOREM 2.

Equations (4.3.2c) *and* (4.3.2d) *hold for all integers* m,n *such that* $m + n > 1$.

Proof: Using the same method as in Theorem 1, the above results can be obtained.

COROLLARY 1.

The ratios of the differences in (4.3.2c),(4.3.2d),(4.3.2e) *and* (4.3.2f) *are constants.*

Proof:

Consider $\dfrac{\Delta R^{i}_{m,n-1}(x)}{\Delta Hg^{i}_{m,n}(x)}$ the ratio of the differences in (4.3.2e). From the proof of Theorem 1 it is clear that the ratio is a constant term (independent of x). The proof for the other ratios follows similary.

COROLLARY 2.

$$Hg^{i}_{m,n}(x) = k_i \; Vg^{i}_{m,n}(x) \quad where \; k_i = - \frac{\Delta Hg^{i}_{m-1,n}(x)}{\Delta Vg^{i}_{m,n-1}(x)}$$

Proof:

This follows immediately by combining (4.3.2c) and (4.3.2d) since the ratios of the differences are inverses and, by Corollary 1,constant.

COROLLARY 3.

In the case $h_j(x) = x^j$ *, the maximum degree,* k, *of the terms* x^k *and* $x^k R^{i}_{m,n}(x)$ *in* $Vg^{i}_{m,n}(x)$ *and* $Hg^{i}_{m,n}(x)$ *are* m *and* n *respectively.*

Proof:

From the initialization (4.3.2a,b) it is clear that the degree of x^k in $Vg^{i}_{m,1-m}(x) = Hg^{i}_{m,1-m}(x)$ is m and the degree, k, of $x^k R$ in $Vg^{i}_{1-n,n}(x) = Hg^{i}_{1-n,n}(x)$ is n. By induction using (4.3.2c,d) and Corollary 1, the maximum degree of x^k in $Vg^{i}_{m,n}(x)$ and $Hg^{i}_{m,n}(x)$ is at most m.Similarly for $x^k R$.

COROLLARY 4. *If* $Hg^{i}_{m,n}(x) = Hg^{i+1}_{m,n}(x)$, *then* $k_i = k_{i+1}$ *(where* k_i *has been defined in Corollary 1) and* $Vg^{i}_{m,n}(x) = Vg^{i+1}_{m,n}(x)$.

Proof: Since $Hg^{i}_{m,n}(x) = Hg^{i+1}_{m,n}(x)$

$$\frac{Hg^{i}_{m-1,n}(x)Vg^{i+1}_{m,n-1}(x) - Hg^{i+1}_{m-1,n}(x)Vg^{i}_{m,n-1}(x)}{Vg^{i+1}_{m,n-1}(x) - Vg^{i}_{m,n-1}(x)}$$

$$= \frac{Hg^{i+1}_{m-1,n}(x)Vg^{i+2}_{m,n-1}(x) - Hg^{i+2}_{m-1,n}(x)Vg^{i+1}_{m,n-1}(x)}{Vg^{i+2}_{m,n-1}(x) - Vg^{i+1}_{m,n-1}(x)}$$

By cross multiplying and inserting $- Vg^{i+1}_{m,n-1}(x)Hg^{i+1}_{m-1,n}(x)$ in both sides, it follows

$$\Delta\, Hg^{i}_{m-1,n}(x)\Delta\, Vg^{i+1}_{m,n-1}(x) = \Delta\, Hg^{i+1}_{m-1,n}(x)\Delta\, Vg^{i}_{m,n-1}(x).$$

Hence $k_i = k_{i+1}$ and by Corollary 1 it follows $Vg^{i}_{m,n}(x) = Vg^{i+1}_{m,n}(x)$.

Note. All these results follow in similar way for the general case when x_i^k is replaced by $h_k(x_i)$ and $x_i^k f_i$ replaced by $h_k(x_i)f_i$.

4.4 THE SINGULAR CASE

These algorithms may break down if the adjacent terms are equal. For example $\Delta\, Hg^{i}_{m,n-1}(x)$ is zero if $Hg^{i+1}_{m,n-1}(x) = Hg^{i}_{m,n-1}(x)$.

Then since $Vg^{i+1}_{m,n-1}(x) = Vg^{i}_{m,n-1}(x)$ from Corollary 4, it follows

$Hg^{i}_{m,n}(x) = \infty$ and $Vg^{i}_{m+1,n-1}(x) = \infty$.

In this discussion it is assumed that such singularities are isolated [cf 12] and correspond loosely to the semi-normal case in Pade approximation. This assumption will be satisfied if the set of given functions form a quasicomplete Chebyshev system on the set of interpolating points [8].

In the case noted above, the indeterminancy of $Hg^{i}_{m,n}(x)$ implies that $\Delta Hg^{j}_{m,n}(x)$ and hence $Hg^{j}_{m+1,n}(x)$ for $j = i-1,i$ cannot be computed. This difficulty may be overcome by jumping two steps. Instead of (4.3.2c) it can be shown

$$Hg^{i}_{m+1,n}(x) = Hg^{i-1}_{m,n}(x) - \Delta g'.Vg^{i-1}_{m+1,n-1}(x) \tag{4.4.1a}$$

$$Hg^{i}_{m+1,n}(x) = Hg^{i+1}_{m,n}(x) - \Delta g.Vg^{i+1}_{m+1,n-1}(x) \tag{4.4.1b}$$

where if m = N,N-1,.....k-n and m+n

$$Hg^{i-1}_{m+1,n}(x) = Hg^{i-1}_{m,n}(x) - \frac{\Delta Hg^{i-1}_{m,n}(x)}{\Delta Vg^{i-1}_{m+1,n-1}(x)} Vg^{i-1}_{m+1,n-1}(x)$$

where

$$\Delta g' = \frac{\Delta Hg^{i-1}_{m,n}(x)}{\Delta Vg^{i-1}_{m+1,n-1}(x)} = \frac{Vg^{i}_{m,n-1}(x)\left(\dfrac{\Delta Hg^{i}_{m-1,n}(x)}{\Delta Vg^{i}_{m,n-1}(x)} - \dfrac{\Delta Hg^{i-1}_{m-1,n}(x)}{\Delta Vg^{i-1}_{m,n-1}(x)}\right)}{Hg^{i}_{m,n-1}(x)\left(\dfrac{\Delta Vg^{i}_{m+1,n-2}(x)}{\Delta Hg^{i}_{m,n-1}(x)} - \dfrac{\Delta Vg^{i-1}_{m+1,n-2}(x)}{\Delta Hg^{i-1}_{m,n-1}(x)}\right)}$$

If $Vg^{i}_{m,n-1}(x) = Hg^{i}_{m,n-1}(x)$ for all i. Then

$$\Delta g' = \frac{\Delta Hg^{i}_{m-1,n}(x) \quad \Delta Vg^{i-1}_{m,n-1}(x) - \Delta Hg^{i-1}_{m-1,n}(x) \quad \Delta Vg^{i}_{m,n-1}(x)}{\Delta Vg^{i}_{m+1,n-2}(x) \ \Delta Hg^{i-1}_{m,n-1}(x) - \Delta Vg^{i-1}_{m+1,n-2}(x) \ \Delta Hg^{i}_{m,n-1}(x)}$$

When $\Delta Hg^{i}_{m,n-1}(x) = \Delta Vg^{i}_{m,n-1}(x) = 0$, the above form can be reduced to

$$\frac{\Delta Hg^{i-1}_{m,n}(x)}{\Delta Vg^{i-1}_{m+1,n-1}(x)} = \frac{\Delta Hg^{i}_{m-1,n}(x)}{\Delta Vg^{i}_{m+1,n-2}(x)}$$

By the same method it can be shown

$$\Delta g = \Delta g' = \frac{\Delta\, Hg^{i}_{m-1,n}(x)}{\Delta\, Vg^{i}_{m+1,n-2}(x)} \tag{4.4.2a}$$

This applies to the case when the singularity occurs at the first step. i.e. $k \neq 2$, otherwise more work is required to derive $\Delta g =$ $\dfrac{\Delta\, Hg^{i}_{m,n}(x)}{\Delta\, Vg^{i}_{m+1,n-1}(x)}$ as follows:

$$\frac{\Delta\, Hg^{i}_{m,n}(x)}{\Delta\, Vg^{i}_{m+1,n-1}(x)} = \frac{Vg^{i+1}_{m,n-1}(x)}{Hg^{i+1}_{m,n-1}(x)}$$

$$\cdot \frac{\Delta\, Hg^{i+1}_{m-1,n}(x)\ \Delta\, Vg^{i}_{m,n-1}(x) - \Delta\, Hg^{i}_{m-1,n}(x)\ \Delta\, Vg^{i+1}_{m,n-1}(x)}{\Delta\, Vg^{i+1}_{m+1,n-2}(x)\ \Delta\, Hg^{i}_{m,n-1}(x) - \Delta\, Vg^{i}_{m+1,n-2}(x)\ \Delta\, Hg^{i+1}_{m,n-1}(x)}$$

$$\cdot \frac{\Delta\, Hg^{i}_{m,n-1}(x)\ \Delta\, Hg^{i+1}_{m,n-1}(x)}{\Delta\, Vg^{i}_{m,n-1}(x)\ \Delta\, Vg^{i+1}_{m,n-1}(x)}$$

where $\dfrac{\Delta\, Hg^{i}_{m,n-1}(x)\ \Delta\, Hg^{i+1}_{m,n-1}(x)}{\Delta\, Vg^{i}_{m,n-1}(x)\ \Delta\, Vg^{i+1}_{m,n-1}(x)}$

$$= \frac{Vg^{i+1}_{m,n-2}(x)\left(\dfrac{\Delta\, Hg^{i}_{m-1,n-1}(x)}{\Delta\, Vg^{i}_{m,n-2}(x)} - \dfrac{\Delta\, Hg^{i+1}_{m-1,n-1}(x)}{\Delta\, Vg^{i+1}_{m,n-2}(x)}\right)}{Hg^{i+1}_{m-1,n-1}(x)\left(\dfrac{\Delta\, Vg^{i}_{m,n-2}(x)}{\Delta\, Hg^{i}_{m-1,n-1}(x)} - \dfrac{\Delta\, Vg^{i+1}_{m,n-2}(x)}{\Delta\, Hg^{i+1}_{m-1,n-1}(x)}\right)}$$

$$\times \frac{Vg^{i+2}_{m,n-2}(x)\left(\dfrac{\Delta\, Hg^{i+1}_{m-1,n-1}(x)}{\Delta\, Vg^{i+1}_{m,n-2}(x)} - \dfrac{\Delta\, Hg^{i+2}_{m-1,n-1}(x)}{\Delta\, Vg^{i+2}_{m,n-2}(x)}\right)}{Hg^{i+2}_{m-1,n-1}(x)\left(\dfrac{\Delta\, Vg^{i+1}_{m,n-2}(x)}{\Delta\, Hg^{i+1}_{m-1,n-1}(x)} - \dfrac{\Delta\, Vg^{i+2}_{m,n-2}(x)}{\Delta\, Hg^{i+2}_{m-1,n-1}(x)}\right)}$$

$$= \frac{Vg^{i+1}_{m,n-2}(x)}{Hg^{i+1}_{m-1,n-1}(x)} \cdot \frac{Vg^{i+2}_{m,n-2}(x)}{Hg^{i+2}_{m-1,n-1}(x)} \cdot \frac{\Delta\ Hg^{i}_{m-1,n-1}(x)}{\Delta\ Vg^{i}_{m,n-2}(x)} \cdot$$

$$\left(\frac{\Delta\ Hg^{i+1}_{m-1,n-1}(x)}{\Delta\ Vg^{i+1}_{m,n-2}(x)}\right)^2 \cdot \frac{\Delta\ Hg^{i+2}_{m-1,n-1}(x)}{\Delta\ Vg^{i+2}_{m-1,n-2}(x)}$$

If $\Delta\ Vg^{i}_{m,n-1}(x) = \Delta\ Hg^{i}_{m,n-1}(x) = 0$, then

$$\frac{\Delta\ Hg^{i}_{m,n}(x)}{\Delta\ Vg^{i}_{m+1,n-1}(x)} = - \frac{\Delta\ Vg^{i+1}_{m,n-2}(x)}{\Delta\ Hg^{i+1}_{m-1,n-1}(x)} \cdot \frac{\Delta\ Hg^{i}_{m-1,n}(x)}{\Delta\ Vg^{i}_{m+1,n-2}(x)} \cdot \frac{\Delta\ Vg^{i+1}_{m,n-1}(x)}{\Delta\ Hg^{i+1}_{m,n-1}(x)} \cdot$$

$$\frac{Vg^{i+1}_{m,n-2}(x)}{Hg^{i+1}_{m-1,n-1}(x)} \cdot \frac{Vg^{i+2}_{m,n-2}(x)}{Hg^{i+2}_{m-1,n-1}(x)} \cdot \frac{\Delta\ Hg^{i}_{m-1,n-1}(x)}{\Delta\ Vg^{i}_{m,n-2}(x)} \cdot$$

$$\left(\frac{\Delta\ Hg^{i+1}_{m-1,n-1}(x)}{\Delta\ Vg^{i+1}_{m,n-2}(x)}\right)^2 \cdot \frac{\Delta\ Hg^{i+2}_{m-1,n-1}(x)}{\Delta\ Vg^{i+2}_{m,n-2}(x)}$$

After the terms rearrangment, these can be expressed as

$$\Delta g = -\Delta_1 . \Delta_2 . \Delta_3 \tag{4,4.2b}$$

where

$$\Delta_1 = \frac{Vg^{i+1}_{m,n-2}(x)}{\Delta\ Vg^{i}_{m+1,n-2}(x)}$$

$$\Delta_2 = \frac{\Delta\ Hg^{i}_{m-1,n}(x)}{Hg^{i+1}_{m-1,n-1}(x)} \cdot \frac{\Delta\ Hg^{i}_{m-1,n-1}(x)}{\Delta\ Vg^{i}_{m,n-2}(x)} \cdot \frac{\Delta\ Hg^{i+1}_{m-1,n-1}(x)}{\Delta\ Vg^{i+1}_{m,n-2}(x)}$$

$$\Delta_3 = \frac{\Delta\ Vg^{i+1}_{m,n-1}(x)}{Hg^{i+2}_{m-1,n-1}(x)} \cdot \frac{Vg^{i+2}_{m,n-2}(x)}{\Delta\ Hg^{i+1}_{m,n-1}(x)} \cdot \frac{\Delta\ Hg^{i+2}_{m-1,n-1}(x)}{\Delta\ Vg^{i+2}_{m,n-2}(x)}$$

and by the same method

$$\Delta_g' = -\Delta_1 . \Delta_2 . \Delta_3' \qquad (4.4.2c)$$

where

$$\Delta_3' = \frac{\Delta\, Vg^{i-1}_{m,n-1}(x)}{Hg^{i}_{m-1,n-1}(x)} \cdot \frac{Vg^{i}_{m,n-2}(x)}{\Delta\, Hg^{i-1}_{m,n-1}(x)} \cdot \frac{\Delta\, Hg^{i-1}_{m-1,n-1}(x)}{\Delta\, Vg^{i-1}_{m,n-2}(x)} \,.$$

if $k = 3,4,\ldots N$

The computation of $Vg^{j}_{m+1,n}(x)$, $j = i-1,i$ may be similarly accomplished by replacing (4.3.2d) by formulas analogous to (4.4.1) with the terms Δg and $\Delta g'$ replaced by $1/\Delta g$ and $1/\Delta g'$ respectively.

All these factors can be shown by the following corollary to be constant terms, and their relation can be shown by Figures 4.4.1 and 4.4.2 .

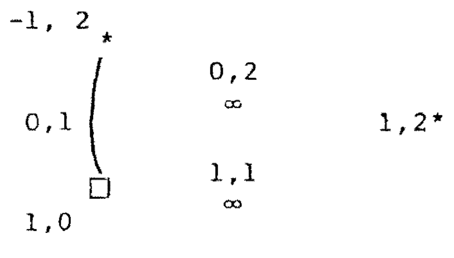

Figure 4.4.1

Singularity occurs

when $\Delta\, Hg^{i}_{1-k,k}(x) = \Delta\, Vg^{i}_{1-k,k}(x) = 0$ for $k = 1,2\ldots$, e.g. $k = 1$

(or $\Delta\, Hg^{i}_{k,1-k}(x) = \Delta\, Vg^{i}_{k,1-k}(x) = 0$)

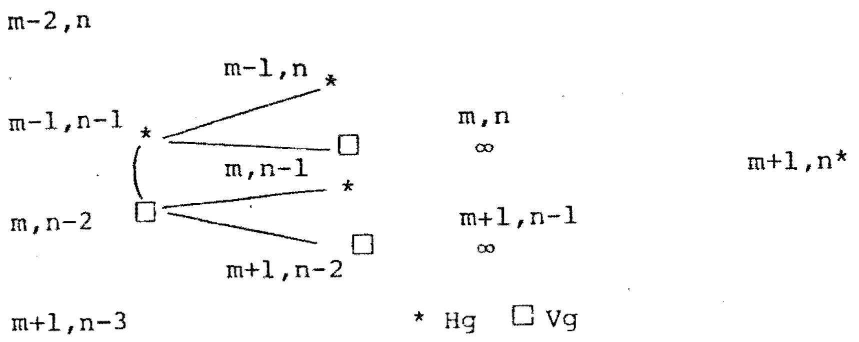

Figure 4.4.2

Singularity occurs

when $\Delta\, Hg^{i}_{m,n-1}(x) = \Delta\, Vg^{i}_{m,n-1}(x) = 0$

If $\Delta Vg^{i}_{0,n-1}(x) = 0$, then $Hg^{i}_{0,n}(x)$ is indeterminate and hence $\Delta Hg^{j}_{0,n}(x)$ and $R^{j}_{0,n}(x)$, $j = i-1,1$, cannot be computed. By using the analogue of (4.4.1) and (4.4.2),

$$R^{i-1}_{0,n}(x) = R^{i-1}_{0,n-1}(x) - \Delta'_R . Hg^{i-1}_{0,n}(x) \qquad (4.4.3a)$$

$$R^{i}_{0,n}(x) = R^{i+1}_{0,n-1}(x) - \Delta_R . Hg^{i+1}_{0,n}(x) \qquad (4.4.3b)$$

where

$$\Delta_R = \Delta'_R = \frac{\Delta R^{i}_{0,n-2}(x)}{\Delta Hg^{\;i}_{-1,n}(x)} \qquad \text{if } n = 2, \text{ and with } m = 0,$$

$$\Delta_R = -\frac{\Delta'_1}{\Delta_2 . \Delta_3} \qquad \text{and}$$

$$\Delta'_R = -\frac{\Delta'_1}{\Delta_2 . \Delta'_3} \qquad \text{if } n = 3,4,\ldots, \text{ and with } m = 0,$$

where

$$\Delta'_1 = \frac{\Delta R^{i}_{0,n-2}(x)}{Vg^{i+1}_{0,n-2}(x)}$$

Figure 4.4.3 shows how the calculation of $R^i_{0,n}(x)$ involves $R^i_{0,n-2}(x)$. Hg and Vg for the connected points in the way

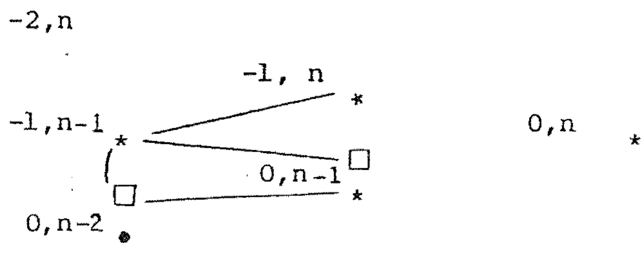

Figure 4.4.3 * Hg □ Vg • R

Similarly, if $\Delta Hg^i_{m-1,0}(x) = 0$, then $R^j_{m,0}(x)$, $j = i-1,i$ may be computed by formulas similar to (4.4.3)

$$R^{i-1}_{m,0}(x) = R^{i-1}_{m-1,0}(x) - \Delta'_R . Vg^{i-1}_{m,0}(x) \qquad (4.4.4a)$$

$$R^{i}_{m,0}(x) = R^{i+1}_{m-1,0}(x) - \Delta_R . Vg^{i+1}_{m,0}(x) \qquad (4.4.4b)$$

where

$$\Delta_R = \Delta'_R = \frac{\Delta R^i_{m-2,0}(x)}{\Delta Vg^i_{m,-1}(x)} \qquad \text{if } m = 2, \text{ and with } n = 0,$$

$$\Delta_R = -\frac{\Delta''_1}{\bar{\Delta}_2 . \bar{\Delta}_3} \quad \text{and}$$

$$\Delta'_R = -\frac{\Delta''_1}{\bar{\Delta}_2 . \bar{\Delta}'_3} \qquad \text{if } m = 3,4,\ldots, \text{ and with } n = 0,$$

where

$$\Delta''_1 = \frac{\Delta R^i_{m-2,0}(x)}{Hg^{i+1}_{m-2,0}(x)}$$

and Δ_2 Δ_3 Δ'_3 may be expressed in the same way as the corresponding expression in (4.4.2b,c) except that $Hg^i_{a,b}(x)$ (resp. $Vg^i_{a,b}(x)$ is replaced by $Vg^i_{b,a}(x)$ (resp. $Hg^i_{b,a}(x)$).

Figure 4.4.4 shows how the calculation of $R^{i}_{m,0}(x)$ involves $R^{i}_{m-2,0}(x)$, Hg and Vg for the connected points in the way

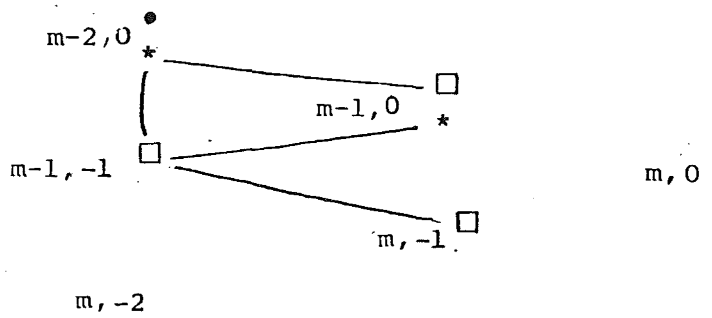

Figure 4.4.4

In fact the above expressions (4.4.3) and (4.4.4) can be generalized to compute $R^{i}_{m,n}(x)$ for m,n = 1,2,3... where some of $R^{i}_{m,n}(x)$ do not exist. But in this case $R^{i}_{m,n}(x)$ may be generated either 'horizontally' or 'vertically' (4.3.2e,f). If the calculation is blocked one way then it is possible to continue in the other way. Thus the situation is simpler than (4.4.3) and (4.4.4).

This approach was motivated by the method used by Wynn [12] to deal with the singular cases.

<u>COROLLARY 5.</u>

For all m,n, the ratios $\Delta g, \Delta g', \Delta_R, \Delta_R'$ *are constants (independent of x)*

[Note that (i) $Vg^{i}_{0,0}(x) = Hg^{i}_{0,0}(x) = 0$

(ii) $Vg^{i}_{m,n}(x)$ $Hg^{i}_{m,n}(x)$ are not defined for $|m| \geq n$ if $m < 0$ or for $|n| \geq m$ if $n < 0$.

(iii) $R^{i}_{m,n}(x)$ are not defined for $m,n < 0$.]

Proof:

Only the first ratio (i.e. $\dfrac{\Delta\, Hg^{i}_{m-1,n}(x)}{Hg^{i+1}_{m-1,n-1}(x)}$) in Δ_2 of (4.4.2b) for m and n $\geqslant$ 0 is proved. The others follow in a similar way.

From (4.3.2g,h),

$$\frac{\Delta\, Hg^{i}_{m-1,n}(x)}{Hg^{i+1}_{m-1,n-1}(x)} = \frac{\dfrac{\begin{vmatrix} -x^{n}f & -x^{n}_{i+1}f_{i+1} & \dots & -x^{n}_{i+m+n-1}f_{i+m+n-1} \\ 1 & 1 & \dots & 1 \\ x & x_{i+1} & \dots & x_{i+m+n-1} \\ \dots & \dots & \dots & \dots \\ x^{m-1} & x^{m-1}_{i+1} & \dots & x^{m-1}_{i+m+n-1} \\ xf & x_{i+1}f_{i+1} & \dots & x_{i+m+n-1}f_{i+m+n-1} \\ \dots & \dots & \dots & \dots \\ x^{n-1}f & x^{n-1}_{i+1}f_{i+1} & \dots & x^{n-1}_{i+m+n-1}f_{i+m+n-1} \end{vmatrix}}{D^{i+1}_{m-1,n}} - \dfrac{\begin{vmatrix} -x^{n}f & -x^{n}_{i}f_{i} & \dots & -x^{n}_{i+m+n-2}f_{i+m+n-2} \\ 1 & 1 & \dots & 1 \\ x & x_{i} & \dots & x_{i+m+n+2} \\ \dots & \dots & \dots & \dots \\ x^{m-1} & x^{m-1}_{i} & \dots & x^{m-1}_{i+m+n-2} \\ xf & x_{i}f_{i} & \dots & x_{i+m+n-2}f_{i+m+n-2} \\ \dots & \dots & \dots & \dots \\ x^{n-1}f & x^{n-1}_{i}f_{i} & \dots & x^{n-1}_{i+m+n-2}f_{i+m+n-2} \end{vmatrix}}{D^{i}_{m-1,n}}}{\dfrac{\begin{vmatrix} -x^{n-1}f & -x^{n-1}_{i+1}f_{i+1} & \dots & -x^{n-1}_{i+m+n-2}f^{n-1}_{i+m+n-2} \\ 1 & 1 & \dots & 1 \\ x & x_{i+1} & \dots & x_{i+m+n-2} \\ \dots & \dots & \dots & \dots \\ x^{m-1} & x^{m-1}_{i+1} & \dots & x^{m-1}_{i+m+n-2} \\ xf & x_{i+1}f_{i+1} & \dots & x_{i+m+n-2}f_{i+m+n-2} \\ \dots & \dots & \dots & \dots \\ x^{n-2}f & x^{n-2}_{i+1}f_{i+1} & \dots & x^{n-2}_{i+m+n-2}f_{i+m+n-2} \end{vmatrix}}{D^{i+1}_{m-1,n-1}}}$$

$$\text{where } D^{i}_{m-1,n} = \begin{vmatrix} 1 & \dots & 1 \\ x_{i} & \dots & x_{i+m+n-2} \\ \dots & \dots & \dots \\ x^{m-1}_{i} & \dots & x^{m-1}_{i+m+n-2} \\ x_{i}f_{i} & \dots & x_{i+m+n-2}f_{i+m+n-2} \\ \dots & \dots & \dots \\ x^{n-1}_{i}f_{i} & \dots & x^{n-1}_{i+m+n-2}f_{i+m+n-2} \end{vmatrix}$$

By applying Sylvester's identity to the determinants and exchanging some rows or columns, then

$$
\frac{\begin{vmatrix}
-x_i^n f_i & -x^n f & -x_{i+1}^n f_{i+1} & \cdots & -x_{i+m+n-1}^n \\
1 & 1 & 1 & \cdots & 1 \\
x_i & x & x_{i+1} & & x_{i+m+n-1} \\
\cdots & \cdots & \cdots & \cdots & \cdots \\
x_i^{m-1} & x^{m-1} & x_{i+1}^{m-1} & \cdots & x_{i+m+n-1}^{m-1} \\
x_i f_i & xf & x_{i+1} f_{i+1} & \cdots & x_{i+m+n-1} f_{i+m+n-1} \\
\cdots & \cdots & \cdots & \cdots & \cdots \\
x_i^{n-1} f_i & x^{n-1} f & x_{i+1}^{n-1} f_{i+1} & \cdots & x_{i+m+n-1}^{n-1} f_{i+m+n-1} \\
0 & 1 & 0 & \cdots & 0
\end{vmatrix}
\begin{vmatrix}
1 & 1 & \cdots & 1 \\
x & x_i & \cdots & x_{i+m+n-2}^{m-1} \\
\cdots & \cdots & \cdots & \cdots \\
x^{m-1} & x_i^{m-1} & \cdots & x_{i+m+n-2}^{m-1} \\
xf & x_i f_i & \cdots & x_{i+m+n-2} f_{i+m+n-2} \\
\cdots & \cdots & \cdots & \cdots \\
x^{n-1} f & x_i^{n-1} f_i & \cdots & x_{i+m+n-2}^{n-1} f_{i+m+n-2}
\end{vmatrix} D_{m-1,n-1}^{i+1}}
{D_{m-1,n}^{i+1} \quad D_{m-1,n}^{i}
\begin{vmatrix}
1 & 1 & \cdots & 1 \\
x & x_i & \cdots & x_{i+m+n-2}^{m-1} \\
\cdots & \cdots & \cdots & \cdots \\
x^{m-1} & x_i^{m-1} & \cdots & x_{i+m+n-2}^{m-1} \\
x f & x_i f_i & \cdots & x_{i+m+n-2} f_{i+m+n-2} \\
\cdots & \cdots & \cdots & \cdots \\
x^{n-1} f & x_i^{n-1} f_i & \cdots & x_{i+m+n-2}^{n-1} f_{i+m+n-2}
\end{vmatrix}}
$$

After eliminating terms this is easily seen to be a constant term.

Using (4.2.3d,e) and the same method it is straightforward to extend the result to the cases $m<0$ or $n<0$.

4.5 NUMERICAL RESULTS

It is obvious that when $x = 0$, this algorithm reduces to the general rational extrapolation. Since the interpolating functions which are generated by this algorithm have the implicit form (refer to the Table below), it may be inconvenient to compute the interpolating function value at a given point, especially when done by the computer. But if this point $x = a$ is transformed to $x' = 0$ and the interpolation algorithm is used, the arithmetic is substantially simplified.

Example 1.

The same example is used as in [4].

Table 4.5.1

Rational interpolating function in an implicit form

i	x_i	$R^i_{0,0}(x)$	$R^i_{0,1}(x)$	$R^i_{0,2}(x)$
0	0	2	$f = -\frac{1}{3}xf+2$	$f = \frac{1}{12}xf - \frac{5}{12}x^2f+2$
1	1	$\frac{3}{2}$	$f = -7xf+12$	$f = -\frac{4}{3}xf - \frac{1}{3}x^2f+4$
2	2	$\frac{4}{5}$	$f = 3xf-4$	$f = \infty$
3	3	$\frac{1}{2}$	$f = \frac{5}{3}xf-2$	$f = \frac{28}{9}xf + \frac{1}{9}x^2f - \frac{14}{3}$
4	4	$\frac{6}{17}$	$f = \frac{37}{29}xf-\frac{714}{493}$	
5	5	$\frac{7}{26}$		

$R^i_{1,0}(x)$	$R^i_{1,1}(x)$	$R^i_{1,2}(x)$
$f = 2-\frac{1}{2}x$	$f = \frac{1}{7}xf+2-\frac{5}{7}x$	$f = -x^2f+2+x$
$f = \frac{11}{5}-\frac{7}{10}x$	$f = -2xf+5-\frac{1}{2}x$	$f = -x^2f+2+x$
$f = \frac{7}{5}-\frac{3}{10}x$	$f = 13xf-22+x$	$f = -x^2f+2+x$
$f = \frac{16}{17}-\frac{5}{34}x$	$f = \frac{14}{5}xf-4+\frac{1}{10}x$	
$f = \frac{152}{221}-\frac{37}{442}x$		

(Continued.)

$R^i_{2,0}(x)$	$R^i_{2,1}(x)$	$R^i_{2,2}(x)$
$f = 2 - \frac{2}{5}x - \frac{1}{10}x^2$	$f = \frac{1}{2}xf+2 - \frac{3}{2}x+\frac{x^2}{4}$	$f = -x^2f+2+x$
$f = \frac{13}{5} - \frac{13}{10}x + \frac{1}{5}x^2$	$f = -\frac{7}{6}xf+4- \frac{5}{6}x+\frac{x^2}{12}$	$f = -x^2f+2+x$
$f = \frac{158}{85} - \frac{58}{85}x + \frac{13}{170}x^2$	$f = -\frac{33}{4}xf+17-\frac{7}{4}x+\frac{x^2}{8}$	
$f = \frac{292}{221} - \frac{163}{442}x + \frac{7}{221}x^2$		
where f is the rational approximation		

These results are exactly the same as those obtained explicitly in [4].

The terms $Hg^i_{m,n}(x)$ and $Vg^i_{m,n}(x)$ for the construction or the interpolating function in the above table can be shown in Table 4.5.2.

Table 4.5.2

i	x_i	f_i	$Hg_{0,1}(x)$		$Hg_{0,2}(x)$	
0	0	2	$-xf$		$xf-x^2f$	
1	1	$\frac{3}{2}$	$-xf+\frac{3}{2}$		$17xf-x^2f-24$	
2	2	$\frac{4}{5}$	$-xf+\frac{8}{5}$		$-13xf-x^2f+24$	
3	3	$\frac{1}{2}$	$-xf+\frac{3}{2}$		$-13xf-x^2f+24$	
4	4	$\frac{6}{17}$	$-xf+\frac{24}{17}$		$-\frac{479}{29}xf-x^2f+\frac{14280}{493}$	
5	5	$\frac{7}{26}$	$-xf+\frac{35}{26}$			

$Vg_{1,0}(x)$	$Hg_{1,1}(x)$	$Vg_{1,1}(x)$	$Hg_{1,2}(x)$	$Vg_{1,2}(x)$
$-x$	$-xf+\frac{3}{2}x$	$\frac{2}{3}xf-x$	$-\frac{1}{7}xf-x^2f+\frac{12}{7}$	$\frac{1}{12}xf+\frac{7}{12}x^2f-x$
$1-x$	$-xf+\frac{7}{5}+\frac{1}{10}x$	$10xf-14-x$	$2xf-x^2f-3+\frac{3}{2}x$	$-\frac{4}{3}xf+\frac{2}{3}x^2f+2-x$
$2-x$	$-xf+\frac{9}{5}-\frac{1}{10}x$	$-10xf+18-x$	$-13xf-x^2f+24$	∞
$3-x$	$-xf+\frac{30}{17}-\frac{3}{34}x$	$-\frac{34}{3}xf+20-x$	$-\frac{14}{5}xf-x^2f+6-\frac{153}{170}x$	$-\frac{476}{153}xf+\frac{170}{153}x^2f-\frac{340}{51}-x$
$4-x$	$-xf+\frac{370}{221}-\frac{29}{442}x$	$-\frac{442}{29}xf+\frac{740}{29}-x$		
$5-x$				

$Vg_{2,0}(x)$	$Hg_{2,1}(x)$	$Vg_{2,1}(x)$	$Hg_{2,2}(x)$	$Vg_{2,2}(x)$
$x-x^2$	$-xf+\frac{11}{5}x-\frac{7}{10}x^2$	$-\frac{10}{7}xf+\frac{22}{7}x-x^2$	$-\frac{1}{2}xf-x^2f+\frac{5}{2}x-\frac{1}{4}x^2$	$-2xf-4x^2f+10x-x^2$
$-2+3x-x^2$	$-xf+\frac{6}{5}+\frac{2}{5}x-\frac{1}{10}x^2$	$-10xf+12+4x-x^2$	$\frac{7}{6}xf-x^2f-2+\frac{11}{6}x-\frac{1}{12}x^2$	$14xf-12x^2f-24+22x-x^2$
$-6+5x-x^2$	$-xf+\frac{156}{85}-\frac{11}{85}x+\frac{1}{170}x^2$	$170xf-312+22x-x^2$	$\frac{33}{4}xf-x^2f-15+\frac{11}{4}x-\frac{1}{8}x^2$	$66xf-8x^2f-120+22x-x^2$
$-12+7x-x^2$	$-xf+\frac{420}{221}-\frac{37}{221}x+\frac{5}{442}x^2$	$\frac{442}{5}xf-168+\frac{74}{5}x-x^2$		
$-20+9x-x^2$				

Numerical rational interpolation at x = 3.5, computed by transforming x = 3.5 to x' = 0.

Table 4.5.3

x'_i	$R_{0,0}$	$R_{0,1}$	$R_{0,2}$
-3.5	2	0.92307692	0.34408602
-2.5	$\frac{3}{2}$	0.47058824	0.45714286
-1.5	$\frac{4}{5}$	0.42105263	∞
-0.5	$\frac{1}{2}$	0.41379310	0.41481481
0.5	$\frac{6}{17}$	0.41791045	
1.5	$\frac{7}{26}$		

$R_{1,0}$	$R_{1,1}$	$R_{1,2}$
0.25	-1.0	0.41509434
-0.25	0.40625	0.41509434
0.35	0.41573034	0.41509434
0.42647059	0.41477273	
0.39479638		

$R_{2,0}$	$R_{2,1}$	$R_{2,2}$
-0.625	0.25	0.41509434
0.5	0.41393443	0.41509434
0.40735294	0.41527197	
0.41855204		

Example 2.

Since $Hg^2_{0,1}(x) = Hg^3_{0,1}(x)$ singularity occurs at $Vg^2_{1,1}(x)$ and $Hg^2_{0,2}(x)$. The approximation $R^2_{0,1}(x)$ does not exist, but by using the rules of Section 4.3 the algorithm can continue to calculate higher order rational approximations.

Table 4.5.4

i	x_i	f_i	$Hg_{0,1}(x)$		$Hg_{0,2}(x)$	
0	0.5	2	$-xf+1$		$\frac{23}{10}xf-x^2f-\frac{9}{5}$	
1	2	3	$-xf+6$		$xf-x^2f+6$	
2	4	0.5	$-xf+2$		∞	
3	1	2	$-xf+2$		$4xf-x^2f+6$	
4	3	2	$-xf+6$			
	$Vg_{1,0}(x)$		$Hg_{1,1}(x)$	$Vg_{1,1}(x)$	$Hg_{1,2}(x)$	$Vg_{1,2}(x)$
	$0.5-x$		$-xf-\frac{2}{3}+\frac{10}{3}x$	$\frac{3}{10}xf+0.2-x$	$\frac{87}{48}xf-x^2f-\frac{51}{24}+\frac{39}{24}x$	$\frac{87}{78}xf-\frac{24}{39}x^2f+\frac{51}{39}-x$
	$2-x$		$-xf+10-2x$	$-\frac{1}{2}xf+5-x$	$2xf-x^2f-4+2x$	$xf-0.5x^2f-2+x$
	$4-x$		$-xf+2$	∞	$3xf-x^2f-6+2x$	$\frac{3}{2}xf-\frac{1}{2}x^2f-3+x$
	$1-x$		$-xf+2x$	$\frac{1}{2}xf-x$		
	$3-x$					

$R^{i}_{m,n}(x)$ can be computed either from $R^{i}_{m-1,n}(x)$ or $R^{i}_{m,n-1}(x)$

Table 4.5.5

i	x_i	$R_{0,0}(x)$	$R_{0,1}(x)$	$R_{0,2}(x)$
0	0.5	2	$f = \frac{1}{5}xf + \frac{9}{5}$	$f = \frac{99}{104}xf - \frac{17}{52}x^2f + \frac{63}{52}$
1	2	3	$f = \frac{5}{8}xf - \frac{6}{8}$	$f = \frac{7}{8}xf - \frac{1}{4}x^2f + \frac{3}{4}$
2	4	0.5	∞	$f = xf - \frac{1}{4}x^2f + \frac{1}{2}$
3	1	2	$f = 2$	
4	3	2		

$R_{1,0}(x)$	$R_{1,1}(x)$	$R_{1,2}(x)$
$f = \frac{5}{3} + \frac{2}{3}x$	$f = \frac{23}{64}xf + \frac{61}{32} - \frac{51}{96}x$	$f = \frac{5}{24}xf + \frac{1}{12}x^2f + \frac{25}{12} - \frac{2}{3}x$
$f = \frac{11}{2} - \frac{5}{4}x$	$f = \frac{3}{8}xf + \frac{7}{4} - \frac{1}{2}x$	$f = \frac{5}{8}xf - \frac{1}{8}x^2f + \frac{5}{4} - \frac{1}{4}x$
$f = \frac{5}{2} - \frac{1}{2}x$	$f = \frac{1}{4}xf + 2 - \frac{1}{2}x$	
$f = 2$		

Example 3.

In this example $f(x_2) = 0$ and hence $R^{i}_{0,1}(x)$, $i = 1,2$ and $R^{i}_{0,2}(x)$, $i = 0,1,2$ do not have an explicit form. In addition $Hg^{0}_{1,1}(x) = Hg^{1}_{1,1}(x)$ and $Vg^{0}_{1,1}(x) = Vg^{1}_{1,1}(x)$ which lead to singularities at $Vg^{0}_{2,1}(x)$ and $Hg^{0}_{1,2}(x)$. Hence $R^{0}_{1,1}(x)$ does not exist. Note that the algorithm continues to calculate higher order interpolations in both cases.

Table 4.5.6

i	x_i	f_i	$Hg_{0,1}(x)$		$Hg_{0,2}(x)$	
0	1	4	$-xf+4$		$-x^2f+4$	
1	2	1	$-xf+2$		$2xf-x^2f$	
2	3	0	$-xf$		$4xf-x^2f$	
3	4	1	$-xf+4$		$-\frac{17}{3}xf+x^2f-\frac{20}{3}$	
4	5	2	$-xf+10$			
	$Vg_{1,0}(x)$		$Hg_{1,1}(x)$	$Vg_{1,1}(x)$	$Hg_{1,2}(x)$	$Vg_{1,2}(x)$
	$1-x$		$-xf+6-2x$	$-\frac{1}{2}xf+3-x$	∞	$-\frac{1}{2}xf+3-x$
	$2-x$		$-xf+6-2x$	$-\frac{1}{2}xf+3-x$	$\frac{10}{3}xf-x^2f-8+\frac{8}{3}x$	$-\frac{5}{4}xf+\frac{3}{8}x^2f+3-x$
	$3-x$		$-xf-12+4x$	$\frac{1}{4}xf+3-x$	$9xf-x^2f+60-2x$	$\frac{9}{20}xf-\frac{1}{20}x^2f+3-x$
	$4-x$		$-xf-20+6x$	$\frac{1}{6}xf+\frac{10}{3}-x$		
	$5-x$					
	$Vg_{2,0}(x)$		$Hg_{2,1}(x)$	$Vg_{2,1}(x)$	$Hg_{2,2}(x)$	$Vg_{2,2}(x)$
	$-2+3x-x^2$		$-xf+6-2x$	∞	$4xf-x^2f-24+14x-2x^2$	$2xf-\frac{1}{2}x^2f-12+7x-x^2$
	$-6+5x-x^2$		$-xf+24-17x+3x^2$	$\frac{1}{3}xf-8+\frac{17}{3}-x^2$	$\frac{1}{2}xf-x^2f+60-\frac{91}{2}x+\frac{17}{2}x^2$	$-\frac{1}{17}xf+\frac{2}{17}x^2f-\frac{120}{17}+\frac{91}{17}x-x^2$
	$-12+7x-x^2$		$-xf-3x+x^3$	$xf+3x-x^2$		
	$-20+9x-x^2$					

Table 4.5.7

i	x_i	$R_{0,0}(x)$	$R_{0,1}(x)$	$R_{0,2}(x)$
0	1	4	$f = -2+\frac{3}{2}xf$	$f = \frac{3}{2}xf-\frac{1}{2}x^2f$
1	2	1	$f = \frac{1}{2}xf$	$f = \frac{3}{4}xf-\frac{1}{8}x^2f$
2	3	0	$f = \frac{1}{4}xf$	$f = \frac{9}{20}xf-\frac{1}{20}x^2f$
3	4	1	$f = \frac{1}{3}+\frac{1}{6}xf$	
4	5	2		

$R_{1,0}(x)$	$R_{1,1}(x)$	$R_{1,2}(x)$
$f = 7-3x$	∞	$f = 2xf-\frac{1}{2}x^2f-3+x$
$f = 3-x$	$f = \frac{1}{3}xf+1-\frac{1}{3}x$	$f = \frac{9}{17}xf-\frac{1}{17}x^2f+\frac{9}{17}-\frac{3}{17}x$
$f = -3+x$	$f = -3+x$	
$f = -3+x$		

$R_{2,0}(x)$	$R_{2,1}(x)$	$R_{2,2}(x)$
$f = 9-6x+x^2$	$f = 9-6x+x^2$	$f = \frac{4}{7}xf-\frac{1}{7}x^2f+\frac{39}{7}-4x+\frac{5}{7}x^2$
$f = 9-6x+x^2$	$f = \frac{1}{2}xf-3+\frac{5}{2}x-\frac{1}{2}x^2$	
$f = -3+x$		

Example 4.

If x_i is considered for $i = 0,1,2,3$ in Example 1, the interpolating functions may be expressed explicitly. Then $R^0_{1,0}(x) = \frac{4-x}{2}$; $R^0_{1,1}(x) = \frac{14-5x}{7-x}$; $R^0_{2,1}(x) = \frac{4-x}{2}$ for the sequence of functions which can be expressed as continued fractions. Note that $x_2 = 2$ is considered as an 'unattainable point' of $R^0_{2,1}(x)$ (see [11]).

If the method suggested in [3] which reorders the points so that the 'unattainable points' appear at the end of the list is used, then

$$R^0_{1,0}(x) = \frac{4-x}{2} \quad \text{and} \quad R^0_{1,1}(x) = \frac{14-5x}{7-x} .$$

In this case $x_3 = 3$ is considered an unattainable point and the algorithm terminates.

With the algorithm described in this chapter, all possible forms of the interpolating function may be computed and decided which is most suitable. Even when more points are added, the interpolation procedure may still be continued without reordering the points and higher order functions may be obtained. For example if $f(4) = \frac{6}{17}$ is added, then $R^0_{2,2}(x) = \frac{2+x}{1+x^2}$ (see Example 1) Alternatively suppose $f(4) = 1$ is added, then $R^0_{2,2}(x) \frac{96-62x+11x^2}{48-22x+4x^2}$. Both of these functions interpolate $f(x)$ at all the points x_i $i = 0,1,2,3,4$ despite the existence of unattainable points for lower order interpolations.

Example 5. (Example 3 in [3]).

If f is infinite at one of the interpolation points, It can be replaced by a parameter α, in the computation.

Suppose $f(0) = 1$, $f(1) = 0$, $f(2) = \infty$. Then

Table 4.5.8

i	x_i	f_i	$Hg_{0,1}(x)$
0	0	1	$-xf$
1	1	0	$-xf$
2	2	α	$-xf+2\alpha$

$Vg_{1,0}(x)$	$Hg_{1,1}(x)$
$-x$	$-xf$
$1-x$	$-xf-2\alpha(1-x)$
$2-x$	

The rational interpolants are

i	$R_{1,0}(x)$	$R_{1,1}(x)$
0	$f = 1-x$	$f = \frac{1+\alpha}{2\alpha}\, xf+1-x$
1	$f = -\alpha(1-x)$	

Hence $R^{0}_{1,1}(x) = \dfrac{1-x}{1-\frac{1}{2}x-\frac{1}{2\alpha}x}$

Setting $\frac{1}{\alpha} = 0$, It is noted that $R^{0}_{1,1}(x) = \dfrac{1-x}{1-\frac{1}{2}x}$ correctly interpolates the data.

4.6 CONCLUSION

An algorithm for the recursive calculation of the interpolating rational function has been given. The algorithm has been constructed in a general form to allow for the expression of the rational function in any suitable basis subject to the Chebyshev condition being satisfied. The algorithm is given a form which lends itself to generalization.

The way of constructing the coefficients of the interpolating function by this algorithm is quite easy, e.g. $R^i_{m,n}(x)$ is obtained either from $R^i_{m-1,n}(x)$ by adding a multiple of $Vg^i_{m,n}(x)$ or from $R^i_{m,n-1}(x)$ by adding a multiple of $Hg^i_{m,n}(x)$. These multiples in fact are the constant ratios of the differences of the adjacent terms of $Vg^i_{m,n}(x)$ or $Hg^i_{m,n}(x)$ even in the singular cases.

It has been shown that an isolated singularity may be avoided by "jumping over" those situations where a rational interpolating function does not exist without the necessity of restarting the calculation for a different ordering of the interpolating points.

The evaluation of the rational interpolating approximation at a particular point $x = a$ is more efficiently accomplished by a transformation.

The general extrapolation algorithm has been derived independently in [4],[5],[9],[10]. The MNA algorithm is quite similar to the algorithm in [9]. The algorithm for rational extrapolation in [9] computes the numerator and denominator separately. The algorithm in this chapter computes the rational extrapolation in an implicit form.

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CHAPTER 5

A GENERAL ALGORITHM FOR PADE APPROXIMATION TO FORMAL POWER SERIES

5.1 INTRODUCTION

A general algorithm for constructing an interpolating function from a linear family of functions forming a Chebyshev system has been given by Brezinski in [1]. This algorithm was extended to generalized rational interpolation in Chapter 4 and is applied to the Pade-type approximants for the series of functions in [1]. A question arises as to whether this algorithm could be extended to generalize the Pade approximation to a formal power series f(x). Before the discussion, some basic definitions are recalled.

The Pade approximant (m,n;x) to a function f(x) which can be expressed as a formal power series $\sum_{k=0}^{\infty} C_k x^k$ is the ratio of Q(m,n;x)/P(m,n;x), where (m,n;x) agrees with the power series as far as possible. The denominator P(m,n;x) and the numerator Q(m,n;x) are polynomials of degree m and n respectively. These polynomials P(m,n;x) and Q(m,n;x) are determined from

$$P(m,n;x) \sum_{k=o}^{\infty} C_k x^k - Q(m,n;x) = O(x^{m+n+1})$$

by neglecting higher order terms. They can be expressed respectively as the quotient of a determinant of order m+l, and its minor whose elements are formed from the Ci.

$$Q(m,n;x) = \frac{\begin{vmatrix} x^m P_0^{n-m}(x) & x^{m-1} P_0^{n-m+1}(x) & \cdots & P_0^n(x) \\ C_{n-m+1} & C_{n-m+2} & \cdots & C_{n+1} \\ \cdots & \cdots & \cdots & \\ C_n & C_{n+1} & \cdots & C_{n+m} \end{vmatrix}}{D_{m,n}} \qquad (5.1.1)$$

where $P_0^i(x) = \sum_{k=0}^{i} C_k x^k$, $C_i = 0$ if $i < 0$ and $D_{m,n}$ is the minor obtained by eliminating the first row and the last column of the numerator.

$P(m,n;x)$ is obtained by replacing $P_0^i(x)$ in (5.1.1) by 1 $\forall$ i.

The Pade table of f(x) is a doubly indexed array of the rational function in (m,n;x). The array is following

$$\begin{array}{lllll} (0,0) & (1,0) & (2,0) & \cdots & (m,0) \\ (0,1) & (1,1) & (2,1) & \cdot\cdot & \\ (0,2) & (1,2) & (2,2) & \cdot & \\ \cdot & \cdot & \cdot & & \\ \cdot & \cdot & & & \\ (0,n) & & & & \end{array}$$

The partial sums of the power series $\sum_{k=0}^{\infty} C_k x^k$ occupy the first column of the table.

A Pade table is normal if none of the (m,n;x) is nil or equal to each other. In other words, the power series f(x) is normal if for each pair (m,n), (m,n;x) agree exactly through the power x^{m+n} and none of the $D_{m,n} = 0$. In particular each coefficient C_i must not vanish. The power series $\sum_{k=0}^{\infty} C_k x^k$ is semi normal if $D_{m,n} = 0$ for m+n even. The nil elements of (m,n;x), if they occur, are isolated by the non-nil elements. Otherwise, the series is called non-normal. More detailed definitions, properties and theorems are given in [6].

Different algorithms for constructing the elements of the Pade table of a power series for the normal case are found in [4]. Some of these algorithms have been modified, in particular situations for the non-normal case [2],[3],[5].

In this chapter, the algorithm for interpolation given by Brezinski in [1] is extended to compute the elements of the Pade table of a power series in the normal case. This algorithm is used to compute separately, column by column, the denominator P(m,n;x) and the numerator Q(m,n;x) of the Pade approximant of f(x). In the next section, how this algorithm can be applied to (5.1.1) will be shown. This algorithm is extended to the seminormal case in Section 5.3. This extension is similar to the method used to solve the singular case in Chapter 4. In the last section some comments are made about the non-normal case.

5.2 THE ALGORITHM

The following algorithm is based on the MNA algorithm in [1]. It is convenient to change some of the notation and initialization. $P_m^n(x)$ is used to compute P(m,n;x) and Q(m,n;x) separately by the same algorithm. Similarly $g_{m,i}^n(x)$ is used to compute $Pg_{m,i}^n(x)$ and $Qg_{m,i}^n(x)$ which are used for computing :(m,n;x) and Q(m,n;x) respectively.

Step 1. Initialization

For $j = 0, 1 \ldots n$

$$P_1^j(x) = \frac{\begin{vmatrix} xP_0^{j-1}(x) & P_0^j(x) \\ C_j & C_{j+1} \end{vmatrix}}{C_j} \tag{5.2.1}$$

For $i = 2, 3 \ldots m$

$$g_{1,i}^j(x) = \frac{\begin{vmatrix} xP_0^{j-1} & x^i P_0^{j-i}(x) \\ C_j & C_{j-i+1} \end{vmatrix}}{C_j}$$

where $P_0^j(x) = \sum_{k=0}^{j} C_k x^k, \ j \geqslant 0$

$= 0 \qquad j < 0$

for computing the numerator $P(m,n;x)$

and $P_0^j(x) = 1, \ \forall j$

for computing the denominator $Q(m,n;x)$

Step 2. For $k = 2, 3 \ldots m.$

$j = 0, 1 \ldots n-1$

$$\text{Compute } P_k^j(x) = \frac{\Delta P_{k-1}(x)}{\Delta g_{k-1,k}^j(x)} \, g_{k-1,k}^j(x) - P_{k-1}^j(x) \tag{5.2.2}$$

If $k = m$ stop, otherwise

$$g_{k,i}^j(x) = \frac{\Delta g_{k-1,i}^j(x)}{\Delta g_{k-1,k}^j(x)} \, g_{k-1,k}^j(x) - g_{k-1,i}^j(x)$$

$$i = k+1, \ldots m \tag{5.2.3}$$

where Δ represents the forward difference on the index j.

$P_k^j(x)$ have the form (5.1.1) if k,j is replaced by m,n and

$$g_{k,i}^j(x) = \frac{\begin{vmatrix} x^kP_0^{j-k}(x) & x^{k-1}P_0^{j-k+1}(x) & \cdots & xP_0^{j-1}(x) & x^iP_0^{j-i}(x) \\ c_{j-k+1} & c_{j-k+2} & \cdots & c_j & c_{j-i+1} \\ \cdot & \cdot & \cdots & \cdot & \cdot \\ c_{j-1} & c_j & \cdots & c^{j+k-2} & c_{j+k-i-1} \end{vmatrix}}{D_{k,j}}$$

The way of computing $g_{k,i}^j(x)$ in (5.2.2) can be generalized as follows. Instead of using $g_{k,i}^j(x)$ for k = 2,3 ...m, we initialize

$$Hg_{2-k,k}^j(x) = -\frac{\begin{vmatrix} x^kP_0^{j-k} & x^{k-1}P_0^{j-k+1} \\ C_{j-k+1} & C_{j-k+2} \end{vmatrix}}{C_{j-k+2}} \qquad j = k-2,k-1,\ldots n.$$

$$Vg_{2-k,k}^j(x) \qquad \frac{\begin{vmatrix} x^kP_0^{j-k} & x^{k-1}P_0^{j-k+1} \\ C_{j-k+1} & C_{j-k+2} \end{vmatrix}}{C_{j-k+1}} \qquad j = k-1,k\ldots n$$

For $\ell = 3,4 \ldots$

  $i = 0,1,2 \ldots$

  $k = i+\ell \ldots m$

  $Hg_{-i,k}^i(x) = -x^kP^{i-k}(x)$

For $j = i+1,\ldots n$

$$\text{Compute } Hg^j_{-i,k}(x) = \frac{\Delta Hg^j_{-(i+1),k}(x)}{\Delta Vg^j_{-i,k-1}(x)} Vg^j_{-i,k-1}(x) - Hg^j_{-(i+1),k}(x) \tag{5.2.4}$$

$$Vg^j_{-i,k}(x) = \frac{\Delta Vg^j_{-i,k-1}(x)}{\Delta Hg^j_{-(i+1),k}(x)} Hg^j_{-(i+1),k}(x) - Vg^j_{-i,k-1}(x) \tag{5.2.5}$$

For $k = 2,3\ldots\ m$

$j = 0,1\ldots\ n-1$

$$\text{Compute } P^j_k(x) = \frac{\Delta P^j_{k-1}(x)}{\Delta Hg^j_{0,k}(x)} Hg^j_{0,k}(x) - P^j_{k-1}(x) \tag{5.2.6}$$

Note: $Vg^j_{-i,k}(x) = 0$ and $Hg^j_{-i,k}(x) = 0$ when $i \geqslant k$

$Hg^j_{0,k}(x) = g^j_{k-1,k}(x)$.

The ratios of the differences in (5.2.2) - (5.2.6) can easily be shown to be constants by using Sylvester's identity (see [7]). Thus the computation is straight-forward. By using this algorithm the Pade table can be built up column by column.

Example: Pade approximants to e^x.

n	$\frac{Q}{P}g^{n}_{1,2}(x)\,(Hg^{n}_{0,2}(x))$	$\frac{Q}{P}g^{n}_{2,3}(x)\,(Hg^{n}_{0,3}(x))$	$\frac{Q}{P}g^{n}_{3,4}(x)\,(Hg^{n}_{0,4}(x))$
0	$\frac{0}{x^2}$	$\frac{0}{x^3}$	$\frac{0}{x^4}$
1	$\frac{-x}{-x+x^2}$	$\frac{2x}{2x-2x^2+x^3}$	$\frac{-6x}{-6x+6x^2-3x^3+x^4}$
2	$\frac{-2x-x^2}{-2x+x^2}$	$\frac{6x+2x^2}{6x-4x^2+x^3}$	$\frac{-24x-6x^2}{-24x+18x^2-6x^3+x^4}$
3	$\frac{-3x+2x^2-\frac{1}{2}x^3}{-3x+x^2}$	$\frac{12x+6x^2+x^3}{12x-6x^2+x^3}$	$\frac{-60x-24x^2-3x^3}{-60x-36x^2-9x^3+x^4}$
4	$\frac{-4x-3x^2-x^3-\frac{1}{6}x^4}{-4x+\frac{1}{24}x^2}$	$\frac{20x+12x^2+3x^3+\frac{1}{3}x^4}{20x-8x^2+x^3}$	$\vdots$
5	$\frac{-5x-4x^2-\frac{1}{2}^3-\frac{1}{3}x^4-\frac{1}{24}x^5}{-5x+x^2}$	$\vdots$	
	$\vdots$		

n	$P^n_1(x)$ (ie. $\frac{Q(1,n;x)}{P(1,n;x)}$)	$P^n_2(x)$	$P^n_3(x)$	$P^n_4(x)$
0	$\frac{1}{1-x}$	$\frac{1}{1-x+\frac{1}{2}x^2}$	$\frac{1}{1-x+\frac{1}{2}x^2-\frac{1}{6}x^3}$	$\frac{1}{1-x+\frac{1}{2}x^2-\frac{1}{6}x^3+\frac{1}{24}x^4}$
1	$\frac{1+\frac{1}{2}x}{1-\frac{1}{2}x}$	$\frac{1+\frac{1}{3}x}{1-\frac{2}{3}x+\frac{1}{6}x^2}$	$\frac{1+\frac{1}{4}x}{1-\frac{3}{4}x+\frac{1}{4}x^2-\frac{1}{24}x^3}$	$\frac{1+\frac{1}{5}x}{1-\frac{4}{5}x+\frac{3}{10}x^2-\frac{1}{15}x^3+\frac{1}{120}x^4}$
2	$\frac{1+\frac{2}{3}x+\frac{1}{6}x^2}{1-\frac{1}{3}x}$	$\frac{1+\frac{1}{2}x+\frac{1}{12}x^2}{1-\frac{1}{2}x+\frac{1}{12}x^2}$	$\frac{1+\frac{2}{5}x+\frac{1}{20}x^2}{1-\frac{3}{5}x+\frac{3}{20}x^2-\frac{1}{60}x^3}$	$\frac{1+\frac{1}{3}x+\frac{1}{30}x^2}{1-\frac{2}{3}x+\frac{1}{5}x^2-\frac{1}{30}x^3+\frac{1}{360}x^4}$
3	$\frac{1+\frac{3}{4}x+\frac{1}{4}x^2+\frac{1}{24}x^3}{1-\frac{1}{4}x}$	$\frac{1+\frac{3}{5}x+\frac{3}{20}x^2+\frac{1}{60}x^3}{1-\frac{2}{5}x+\frac{1}{20}x^2}$	$\frac{1+\frac{1}{2}x+\frac{1}{10}x^2+\frac{1}{120}x^3}{1-\frac{1}{2}x+\frac{1}{10}x^2-\frac{1}{120}x^3}$	$\vdots$
4	$\frac{1+\frac{4}{5}x+\frac{3}{10}x^2+\frac{1}{15}x^3+\frac{1}{120}x^4}{1-\frac{1}{5}x}$	$\frac{1+\frac{2}{3}x+\frac{1}{5}x^2+\frac{1}{30}x^3+\frac{1}{360}x^4}{1-\frac{1}{3}x+\frac{1}{30}x^2}$	$\vdots$	
5	$\frac{1+\frac{5}{6}x+\frac{1}{3}x^2+\frac{1}{12}x^3+\frac{1}{72}x^4+\frac{1}{720}x^5}{1-\frac{1}{6}x}$	$\vdots$		

5.3 SEMI-NORMAL CASE

The above algorithm may break down if $C_i = 0$ in (5.2.1) or $\Delta g^j_{k-1,k}(x) = 0$ in (5.2.2 - 5.2.3) or $\Delta Hg^j_{-i,k}(x)$ (or $\Delta Vg^j_{-i,k}(x)) = 0$ in (5.2.4 - 5.2.6). For the semi-normal case, the extension of (5.2.4 - 5.2.6) allows the recursive algorithm to carry on.

If $\Delta Vg^j_{-i,k-1}(x) = 0$ and $\Delta Hg^j_{-i,k-1}(x) = 0$ (refer to Cor. 4 in Chapter 4) in (5.2.4), $Hg_{-i,k}(x)$, $Vg^j_{-(i-1),k-1}(x)$ and $P^j_{k-1}(x)$ cannot be computed. Next a step is jumped to compute $Hg^{j-1}_{-(i-1),k}(x)$, $Hg^j_{-(i-1),k}(x)$, $Vg^{j-1}_{-(i-1),k}(x)$, $Vg^j_{-(i-1),k}(x)$, $P^{j-1}_k(x)$ and $P^j_k(x)$ by the following

a) $$Hg^{j-1}_{-(i-1),k}(x) = \Delta' g \; Vg^{j-1}_{-(i-1),k-1}(x) - Hg^{j-1}_{-i,k}(x)$$

$$Vg^{j-1}_{-(i-1),k}(x) = \frac{1}{\Delta' g} Hg^{j-1}_{-i,k}(x) - Vg^{j-1}_{-(i-1),k-1}(x)$$

$$Hg^{j}_{-(i-1),k}(x) = \Delta g \; Vg^{j+1}_{-(i-1),k-1}(x) - Hg^{j+1}_{-i,k}(x)$$

$$Vg^{j}_{-(i-1),k}(x) = \frac{1}{\Delta g} Hg^{j+1}_{-i,k}(x) - Vg^{j+1}_{-(i-1),k-1}(x) \quad i = 1,2 \ldots$$

where $\Delta g = \Delta' g = \dfrac{C_{j-k+1}}{C_{j-k+3}}$ for $k = i+3$.

$$\Delta g = -\Delta_1 \cdot \Delta_2 \cdot \Delta_3 \quad \text{for } k = i+4,\ i+5 \ldots$$

where $$\Delta_1 = \frac{Vg_{-i,k-2}(x)}{\Delta Vg^j_{-(i-1),k-2}(x)}$$

$$\Delta_2 = \frac{\Delta Hg^j_{-(i+1),k}(x)}{Hg^{j+1}_{-(i+1),k-1}(x)} \cdot \frac{\Delta Hg^j_{-(i+1),k-1}(x)}{\Delta Vg^j_{-i,k-2}(x)} \cdot \frac{\Delta Hg^{j+1}_{-(i+1),k-1}(x)}{\Delta Vg^{k+1}_{-i,k-2}(x)}$$

$$\Delta_3 = \frac{\Delta Hg^{j+2}_{-(i+1),k-1}(x)}{\Delta Vg^{j+2}_{-i,k-2}(x)} \cdot \frac{\Delta Vg^{j+1}_{-i,k-1}(x)}{Hg^{j+2}_{-(i+1)k-1}(x)} \cdot \frac{Vg^{j+2}_{-i,k-2}(x)}{\Delta Hg^{j+1}_{-i,k-1}(x)}$$

and by the same method, we have

$$\Delta' g = -\Delta_1 \cdot \Delta_2 \cdot \Delta_3'$$

where $\Delta_3' = \dfrac{\Delta Hg^{j-1}_{-(i+1),k-1}(x)}{\Delta Vg^{j-1}_{-i,k-2}(x)} \cdot \dfrac{\Delta Vg^{j-1}_{-i,k-1}(x)}{Hg^{j}_{-(i+1),k-1}(x)} \cdot \dfrac{Vg^{j}_{-i,k-2}(x)}{\Delta Hg^{j-1}_{-i,k-1}(x)}$

b) $P^{j-1}_k(x) = \Delta_P' \, Hg^{j-1}_{0,k}(x) - P^{j-1}_{k-1}(x)$

$$P^j_k(x) = \Delta_P \, Hg^{j+1}_{0,k}(x) - P^{j+1}_{k-1}(x)$$

where $\Delta_P = \Delta_P' = \dfrac{C_{j+1}}{C_{j-1}}$ for $k = 2$.

$$\Delta_P = -\Delta_1' \frac{1}{\Delta_2 . \Delta_3}$$

and $\Delta_P' = -\Delta_1' \dfrac{1}{\Delta_2 . \Delta_3'}$

where $\Delta_1' = \dfrac{\Delta P^j_{k-2}(x)}{Vg^{j+1}_{0,k-2}(x)}$ for $k = 3,4 \ldots$

A more detailed theoretical derivation is given in [7]. The idea of this extension is similar to Theorem 7.4 of [6].

5.4 NON-NORMAL CASE

For the non-normal case, the nil elements appear in the Pade table more than once. Hence it will be more complicated to generalize. An algorithm and some techniques for computing the non-normal staircase Pade table can be found in [3] , [5] . For the more general scheme, perhaps we can apply the general Neville-Aitken algorithm in [1] . That is

$$P^j_{k+m}(x) = \frac{\begin{vmatrix} P^j_m(x) & \cdots & P^{j+k}_m(x) \\ g^j_{m,m+1}(x) & \cdots & g^{j+k}_{m,m+1}(x) \\ \cdots & \cdots & \cdots \\ g^j_{m,m+k}(x) & \cdots & g^{j+k}_{m,m+k}(x) \end{vmatrix}}{\begin{vmatrix} 1 & \cdots & 1 \\ g^j_{m,m+1}(x) & & g^{j+k}_{m,m+1}(x) \\ \cdots & \cdots & \cdots \\ g^j_{m,m+k}(x) & \cdots & g^{j+k}_{m,m+k}(x) \end{vmatrix}} = \frac{\begin{vmatrix} P^j_k(x) & \cdots & P^{j+m}_k(x) \\ g^j_{k,k+1}(x) & \cdots & g^{j+m}_{k,k+1}(x) \\ \cdots & \cdots & \cdots \\ g^j_{k,k+m}(x) & \cdots & g^{j+m}_{k,k+m}(x) \end{vmatrix}}{\begin{vmatrix} 1 & \cdots & 1 \\ g^j_{k,k+1}(x) & & g^{j+m}_{k,k+1}(x) \\ \cdots & \cdots & \cdots \\ g^j_{k,k+m}(x) & \cdots & g^{j+m}_{k,k+m}(x) \end{vmatrix}}$$

This relation holds for $g^j_{k+m,i}(x)$ if we replace the first row in the numerators by $(g^j_{m,i}(x) \ \ldots \ g^{j+k}_{m,i}(x))$ and $(g^j_{k,i}(x) \ \ldots \ g^{j+m}_{k,i}(x))$ respectively where $k,m = 1,2 \ldots$ It can be used in the semi-normal case when $m = 2$ in the second relation, but for $m > 2$, we have to evaluate a larger determinant. The simplification of the computation for more general non-normal cases is still being studied.

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CHAPTER 6

THE QUADRATIC APPROXIMATION

6.1 INTRODUCTION

Pade approximations are widely used for solving problems more efficiently and accurately than polynomial approximations. In recent years, there has been some interest in generalizations and extensions of Pade approximations. The Pade approximation has been extended to quadratic approximation [10] and used in applications to approximate certain functions with branch points [6],[11]. Some of these results show that the quadratic approximation provides a better approximation than the Pade approximation. In this chapter the quadratic approximation has been studied. The general forms of expressing the quadratic approximation by the polynomial coefficients are defined in the next section and the identities among these polynomial coefficients are shown in section 6.3. A general algorithm for computing these polynomial coefficients is given in section 6.4. This algorithm is an extension of the MNA-algorithm [2]. Naturally this approximation can be applied to accelerate the convergence of a sequence and this is discussed in section 6.5. Furthermore, this idea may be applied to interpolation. If quadratic approximation is a three-dimensional analogue of the two dimensional Pade approximation [10], then quadratic interpolation is a three-dimensional analogue of the two dimensional rational interpolation. The general algorithm for rational interpolation in [7] is extended to quadratic interpolation in section 6.6. The interpolating value at $x_i = 0$ will reduce the interpolation to extrapolation and it can be applied to extrapolate numerical integration. Some numerical results by using quadratic approximation and quadratic interpolation are presented in section 6.7

6.2 QUADRATIC APPROXIMATION

To extend the Pade approximation to the quadratic case the approximant of the function f(x) which can be expressed as a formal power series $\sum_{i=0}^{\infty} c_i x^i$ should be considered as a root of a quadratic equation:

$$\alpha(\ell,m,n;x)f^2(x) + \beta(\ell,m,n;x)f(x) + \gamma(\ell,m,n;x) = 0 \qquad (6.2.1)$$

where
$$\alpha(\ell,m,n;x) = \sum_{i=0}^{\ell} a_i x^i$$

$$\beta(\ell,m,n;x) = \sum_{i=0}^{m} b_i x^i$$

$$\gamma(\ell,m,n;x) = \sum_{i=0}^{n} \gamma_i x^i$$

are the polynomial coefficients of the quadratic approximation of f(x). $(\ell,m,n;x)$ is the quadratic approximant of f(x) in (6.2.1).

The accuracy of the approximation of f(x) is $0(x^{\ell+m+n+2})$ since the higher order terms are neglected.

If the condition $a_0 = 1$ (or $b_0 = 1$) is imposed, then the coefficients, a_i, b_i, γ_i can be determined by $(\ell+m+n+2)$ linear equations which equate like powers of x.

$$
\begin{aligned}
\text{i.e.}\quad x^0 &: \quad A_0 + C_0 b_0 + \gamma_0 = 0 \\
x^1 &: \quad A_1 + a_1 A_0 + b_0 C_1 + b_1 C_0 + \gamma_1 = 0 \\
x^2 &: \quad A_2 + a_1 A_1 + a_2 A_0 + b_0 C_2 + b_1 C_1 + b_2 C_0 + \gamma_2 = 0 \\
&\ \ \vdots \\
x^n &: \quad A_n + a_1 A_{n-1} + \cdots + a_\ell A_{n-\ell} + b_0 C_n + \cdots + b_m C_{n-m} + \gamma_n = 0 \\
x^{n+1} &: \quad A_{n+1} + a_1 A_n + \cdots + a_\ell A_{n-\ell+1} + b_0 C_{n+1} + b_1 C_n + \cdots + b_m C_{n-m+1} = 0 \\
&\ \ \vdots \\
x^{\ell+m+n+1} &: \quad A_{\ell+m+n+1} + a_1 A_{\ell+m+n} + \cdots + a_\ell A_{m+n+1} + b_0 C_{\ell+m+n+1} + b_1 C_{\ell+m+n} \\
&\qquad + \cdots + b_m C_{\ell+n+1} = 0
\end{aligned}
$$

where A_i is the coefficient of x^i in the square of $\sum_{i=0}^{\infty} C_i x^i$

$$a_i = 0 \quad \text{if} \quad i > \ell$$

$$b_i = 0 \quad \text{if} \quad i > m$$

and

$$A_i = 0 \quad \text{if} \quad i < 0$$

$$C_i = 0 \quad \text{if} \quad i < 0 \quad .$$

These polynomial coefficients $\alpha(\ell,m,n,;x)$, $\beta(\ell,m,n;x)$ and $\gamma(\ell,m,n;x)$ can be expressed respectively as the quotient of a determinant of order $\ell+m+2$ and its minor whose elements are formed from the C_i and A_i.

$P(\ell,m,n;x) =$

$$
\frac{(-1)^{\ell+m+1}\begin{vmatrix} x^m p^{n-m}(x) & x^{m-1}p^{n-m+1}(x) & \cdots & p^n(x) & x^\ell q^{n-\ell}(x) & x^{\ell-1}q^{n-\ell+1}(x) & \cdots & q^n(x) \\ C_{n-m+1} & C_{n-m+2} & \cdots & C_{n+1} & A_{n-\ell+1} & A_{n-\ell+2} & \cdots & A_{n+1} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ C_{\ell+n+1} & C_{\ell+n+2} & \cdots & C_{\ell+m+n+1} & A_{m+n+1} & A_{m+n+2} & \cdots & A_{\ell+m+n+1} \end{vmatrix}}{D} \tag{6.2.2}
$$

$$\left.\begin{array}{ll}\text{For } P = \alpha: & p^i(x) = 0, \quad q^i(x) = 1 \\ P = \beta: & p^i(x) = 1, \quad q^i(x) = 0\end{array}\right\} \forall\ i$$

$$P = \gamma: \ p^i(x) = -\sum_{K=0}^{i} C_K x^K, \ q^i(x) = -\sum_{K=0}^{i} A_K x^K$$

where D is the minor obtained by eliminating the first row and the last column of the numerator. For reasons of simplicity in presentation, all D are assumed different from zero. Since α,β,γ have same sign we ignore $(-1)^{\ell+m+1}$ during the computation.

The approximant of f(x) is a root of the quadratic equation (6.2.1). A question may arise immediately as to how the root is selected. For finding zeros of a function, one could select the root closest to zero (Cauchy's Method) and hence take $(-\beta + \sqrt{\beta^2 - 4\alpha\gamma})/2\alpha = -2\gamma/(\beta + \sqrt{\beta^2 - 4\alpha\gamma})$ [10]. But for the other purposes, such as extrapolation, the root closest to the extrapolating point is selected. This is the procedure for the numerical results from section 6.7. These results show the approximant shifts between two roots of the quadratic equation. It cannot be decided which one will be the approximant we want until the roots are found. Then the root closer to the previous approximation is chosen.

6.3 IDENTITIES AMONG THE POLYNOMIAL COEFFICIENTS OF THE QUADRATIC APPROXIMATION

In the quadratic polynomial coefficients $P(\ell,m,n;x)$ ℓ, m and n are the highest degrees of the polynomial $\alpha(\ell,m,n;x)$, $\beta(\ell,m,n;x)$ and $\gamma(\ell,m\,n;x)$ respectively. For the zero degree, the coefficient of x^0 still exists. For example $(0,0,1;x)$ means

$f^2(x) + b_0 f(x) + (\gamma_0 + \gamma_1 x) = 0$ (we assume $a_0 = 1$). Since the polynomial coefficients have common denominators, the denominators are temporarily omitted and the relationships among the numerators are derived.

Let $N(m,n;x)$ and $D(m,n;x)$ be the numerator and denominator of the Pade approximant $(m,n;x)$ of $f(x) = \sum_{i=0}^{\infty} C_i x^i$. From [5] the identities are as follows,

$$\begin{matrix} N \\ D \end{matrix}(m,n;x) = \left\{ \begin{matrix} N \\ D \end{matrix}(m-1;n-1;x) \times \begin{matrix} N \\ D \end{matrix}(m-1,n+1;x) - \begin{matrix} N \\ D \end{matrix}(m-1,n;x)^2 \right\} \Big/ \begin{matrix} N \\ D \end{matrix}(m-2,n;x) \quad \text{for } m = 1,2\ldots,\ n = 0,1\ldots. \tag{6.3.1}$$

and

$$D(1,n;x) = C_{n+1}\,x - C_n \quad \text{(since } D(1,n;x) \text{ is not defined in the above expression)}$$

where

$$\begin{matrix} N \\ D \end{matrix}(0,n;x) = \begin{matrix} \sum_{i=0}^{n} C_i x^i \\ 1 \end{matrix}$$

$$\begin{matrix} N \\ D \end{matrix}(m,-1;x) = \begin{matrix} 0 \\ (-C_0 x)^m \end{matrix} \qquad m \geq 0$$

$$\begin{matrix} N \\ D \end{matrix}(-1,n;x) = \begin{matrix} x^n \\ 0 \end{matrix} \qquad n \geq 0$$

Using the notation P' to distinguish the numerator part of P, and from (6.2.2) $P'(0,0,n;x) = A_{n+1}\,p^n(x) - C_{n+1}q^n(x)$.

The Sylvester determinant identity is used to decompose $P'(0,m,n;x)$ and the following relations are obtained by using identity (6.3.1)

$$\alpha'(0,m,n;x) = \left\{\alpha'(0,m-1,n-1;x) \times \alpha'(0,m-1,n+1;x) - \alpha'(0,m-1,n;x)^2\right\} \Big/ \alpha'(0,m-2,n;x)$$

$$\begin{matrix}\beta'\\ \gamma'\end{matrix}(0,m,n;x) = \left\{ \begin{matrix}D\\N\end{matrix}(m,n;x) \times \begin{matrix}\beta'\\ \gamma'\end{matrix}(0,m-1,n+1;x) - \begin{matrix}D\\N\end{matrix}(m,n+1;x)\ \begin{matrix}\beta'\\ \gamma'\end{matrix}(0,m-1,n;x)\right\} \Big/ \begin{matrix}D\\N\end{matrix}(m-1,n+1;x) \quad \text{where } m=1,2,3\ldots n=0,1,2\ldots$$

and

$$\alpha'(0,-1,n;x) = 1, \quad \alpha'(0,m,-1;x) = -C_0^{m+1} \qquad (6.3.2a)$$

Similarly, let $AN(\ell,n;x)$ and $AD(\ell,n;x)$ be the numerator and denominator of the Pade approximant $(\ell,n;x)$ of $\sum_{i=0}^{\infty} A_i x^i$ then these also satisfy identity (6.3.1).

$$\beta'(\ell,0,n;x) = \left\{\beta'(\ell-1,0,n-1;x) \times \beta'(\ell-1,0,n+1,;x) - \beta'(\ell-1,0,n;x)^2\right\} \Big/ \beta'(\ell-2,0,n;x)$$

$$\begin{matrix}\alpha'\\ \gamma'\end{matrix}(\ell,0,n;x) = \left\{\begin{matrix}AD\\AN\end{matrix}(\ell,n+1;x) \times \begin{matrix}\alpha'\\ \gamma'\end{matrix}(\ell-1,0,n;x) - \begin{matrix}AD\\AN\end{matrix}(\ell,n;x) \times \begin{matrix}\alpha'\\ \gamma'\end{matrix}(\ell-1,0,n+1;x)\right\} \Big/ \begin{matrix}AD\\AN\end{matrix}(\ell-1,n+1;x)$$

where $\ell = 1,2,3\ldots n = 0,1,2\ldots.$ (6.3.2b)

and $\beta'(-1,0,n;x) = 1, \quad \beta'(\ell,0,-1;x) = -A_0^{\ell+1}$.

Now except for $\alpha'(0,m,n;x)$ and $\beta'(\ell,0,n;x)$, a more general form to express the relationship of these coefficient polynomials is the following

For $\ell = 1,2\ldots, \quad m,n = 0,1,2\ldots$

or $m = 1,2\ldots, \quad \ell,n = 0,1,2\ldots$

$$P'(\ell,m,n;x) = \left\{P'(\ell-1,m,n;x) \times P'(\ell,m-1,n+1;x) - P'(\ell,m-1,n;x) \times P'(\ell-1,m,n+1;x)\right\} \Big/ P'(\ell-1,m-1,n+1;x) \qquad (6.3.3)$$

where $$\frac{\alpha'}{\gamma'}(\ell,-1,n;x) = \frac{AD}{AN}(\ell,n;x)$$

$$\frac{\beta'}{\gamma'}(-1,m,n;x) = \frac{D}{N}(m,n;x)$$

Note that since $a_0 = 1$ $\alpha(0,m,n;x) = 1$ and hence division by $\alpha'(0,m,n;x)$ will give the required normalization. The relationship between the different $P(\ell,m,n;x)$ is shown in Figure (6.3.1)

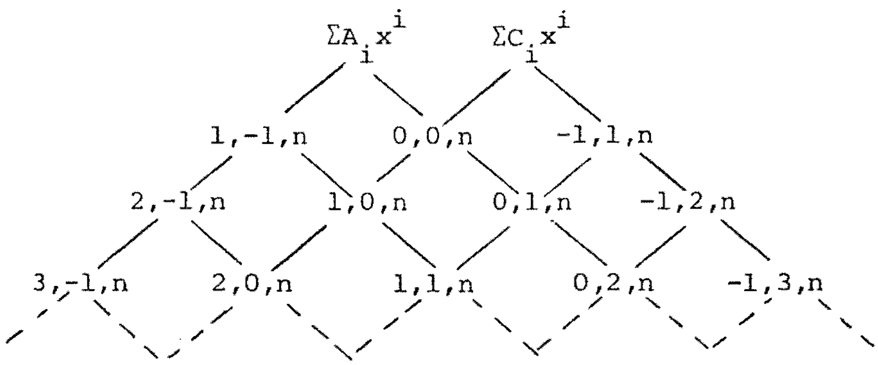


Figure 6.3.1

6.4 THE GENERAL ALGORITHM FOR THE POLYNOMIAL COEFFICIENTS OF THE QUADRATIC APPROXIMATION

(6.2.1) can be solved by using $P'(\ell,m,n;x)$ which can be computed recursively from (6.3.1) - (6.3.3). Since it involves the product of two terms, when the approximation is evaluated it may cause overflow or underflow during the computation if the multiple is too large or too small. Fortunately, a general recursive procedure - MNA algorithm - has recently been found by Brezinski [2] and it has been extended to the rational interpolation [7][8] and Pade approximation [9]. By the analogue of this algorithm, the quadratic polynomial coefficients of the quadratic approximation of f(x) can be computed recursively and effectively in a more general way. Each polynomial coefficient is computed in turn.

Suppose the partial sum $\sum_{i=0}^{n} C_i x^i$ of $f(x) = \sum_{i=0}^{\infty} C_i x^i$ is given. The polynomial coefficients $P(\ell,m,n;x)$, $\ell,m,n \geqslant 0$ of the quadratic approximation of $f(x)$ can be computed by the following algorithm.

A. Basic formulas:

For convenience, $Pg_i(\ell,m,n;x)$ are defined for computing $P(\ell,m,n;x)$ from $P(\ell-1,m,n;x)$ if $i = 1$ and from $P(\ell,m-1,n;x)$ if $i = 2$. Note that when $P = \alpha$ then Pg is to be interpreted as αg and similarly for $P = \beta,\gamma$. The $Pg^n_{\ell,j}(x)$ and $Qg^n_{\ell,j}(x)$ are intermediate stages in the computation of $Pg_1(\ell,0,n;x)$ and $Pg_2(0,\ell,n;x)$ respectively. These intermediate polynomials are both computed by the MNA algorithm [2] (equation 6.4.1).

$$Pg^n_{\ell,j}(x) = \frac{\Delta\gamma g^n_{\ell-1,j}(x)}{\Delta\gamma g^n_{\ell-1,\ell}(x)} \; Pg^n_{\ell-1,\ell}(x) - Pg^n_{\ell-1,j}(x) \tag{6.4.1}$$

$$Pg_1(\ell,m,n;x) = \frac{\Delta\gamma g_1(\ell,m-1,n;x)}{\Delta\gamma g_2(\ell-1,m,n;x)} \; Pg_2(\ell-1,m,n;x) - Pg_1(\ell,m-1,n;x) \tag{6.4.2}$$

$$Pg_2(\ell,m,n;x) = \frac{\Delta\gamma g_2(\ell-1,m,n;x)}{\Delta\gamma g_1(\ell,m-1,n;x)} \; Pg_1(\ell, m-1,n;x) - Pg_2(\ell-1,m,n;x) \tag{6.4.3}$$

$$P(\ell,m,n;x) = \frac{\Delta\gamma(\ell-1,m,n;x)}{\Delta\gamma g_1(\ell,m,n;x)} \; Pg_1(\ell,m,n;x) - P(\ell-1,m,n;x) \tag{6.4.4}$$

$$P(\ell,m,n;x) = \frac{\Delta\gamma(\ell,m-1,n;x)}{\Delta\gamma g_2(\ell,m,n;x)} \; Pg_2(\ell,m,n;x) - P(\ell,m-1,n;x) \tag{6.4.5}$$

where Δ represents the forward difference on the index n.

B. The Algorithms:

Algorithm I

Step 1. For $\ell = 1$; $n = 0,1,\ldots,N-1$,

initialize $$Pg_1(1,0,n;x) = Qg^n_{1,2}(x) = \frac{\begin{vmatrix} p^n(x) & xq^{n-1}(x) \\ C_{n+1} & A_n \end{vmatrix}}{C_{n+1}}$$

$$Pg_2(0,1,n;x) = Pg^n_{1,2}(x) = -\frac{\begin{vmatrix} xp^{n-1}(x) & p^n(x) \\ C_n & C_{n+1} \end{vmatrix}}{C_{n+1}}$$

$$P(0,0,n;x) = \frac{\begin{vmatrix} p^n(x) & q^n(x) \\ C_{n+1} & A_{n+1} \end{vmatrix}}{C_{n+1}}$$

Step 2. For $n = 0,1\ldots N-2$;

Compute $P(1,0,n;x)$ by (6.4.4) and $P(0,1,n;x)$ by (6.4.5).

Define $NT = N$.

Step 3. Termination criterion.

If $\ell = NT - 2$ stop.

$\ell = \ell+1$ otherwise.

Step 4. $j = \ell+1$; Set $N = NT$.

For $n = 1,\ldots\ldots N-1$,

initialize $$Qg^n_{1,j}(x) = \frac{\begin{vmatrix} p^n(x) & x^{j-1}q^{n-j+1}(x) \\ C_{n+1} & A_{n-j+2} \end{vmatrix}}{C_{n+1}}$$

$$Pg^n_{1,j}(x) = -\frac{\begin{vmatrix} x^{j-1}p^{n-j+1}(x) & p^n(x) \\ C_{n-j+2} & C_{n+1} \end{vmatrix}}{C_{n+1}}$$

Step 5. Set $N = N - 1$.

For $k = 2\ldots\ell$; $n = 0,1\ldots N-1$;

Compute $Qg^n_{k,j}(x)$ and $Pg^n_{k,j}(x)$ by (6.4.1).

then define $Pg_1(\ell,0,n;x) = Qg^n_{\ell,\ell+1}(x)$

$$Pg_2(0,\ell,n;x) = Pg^n_{\ell,\ell+1}(x).$$

Step 6. For $n = 0,1\ldots N-2$;

Compute $P(\ell,0,n;x)$ by (6.4.4) and $P(0,\ell,n;x)$ by (6.4.5).

Step 7. Set $N = N - 1$.

For $j = \ell, \ell-1\ldots1$; $n = 0,1\ldots N-1$; $i = 1,2$;

Compute $Pg_i(j,(\ell+1)-j,n;x)$ by (6.4.2) and (6.4.3).

Step 8. For $j = \ell, \ell-1\ldots1$; $n = 0,1\ldots N-2$;

Compute $P(j,(\ell+1)-j,n;x)$ by (6.4.4) or (6.4.5).

Go to step 3.

The steps of the algorithm can be seen from the following diagram (figure 6.4.1).

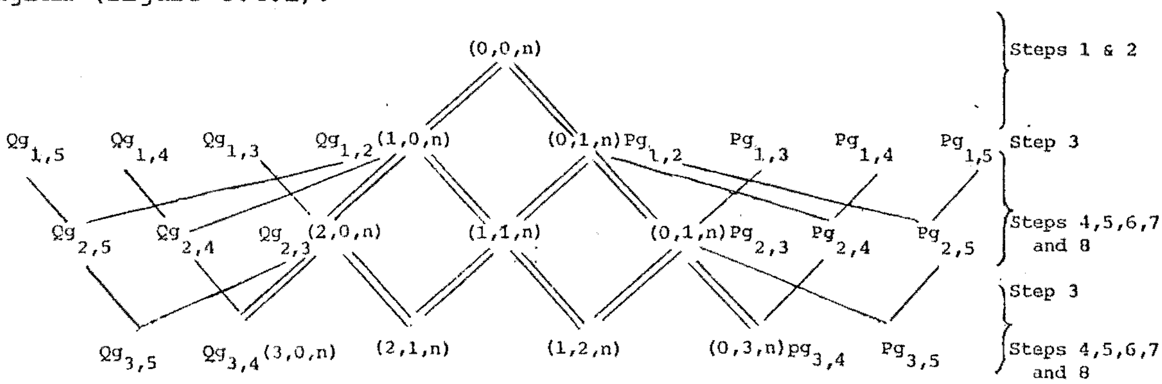


Figure 6.4.1

$P(\ell,m,n;x)$ is computed in the double lined area

The initializations and computations of $Qg^n_{k,j}(x)$ and $Pg^n_{k,j}(x)$ in Steps 4 and 5 are similar to that in the MNA algorithm [2] which is based on Aitken's pattern while the computation of $Pg_i\ (\ell,m,n;x)$ in Step 7 is based on Neville's pattern [7]. Steps 4 and 5 can be unified in the same way as Step 7 as follows.

Algorithm II

Steps 1 and 2. Same as Algorithm I.

Step 3. If ℓ = NT - 2 stop.

Step 4. Set N = NT.

For $n = \ell-1 \ldots N-1$,

initialize
$$Pg_2(\ell,1-\ell,n;x) = -\frac{\begin{vmatrix} x^{\ell-1}q^{n-\ell+1}(x) & x^{\ell}q^{n-\ell}(x) \\ A_{n-\ell+2} & A_{n-\ell+1} \end{vmatrix}}{A_{n-\ell+1}}$$

$$Pg_1(1-\ell,\ell,n;x) = \frac{\begin{vmatrix} x^{\ell}p^{n-\ell}(x) & x^{\ell-1}p^{n-\ell+1}(x) \\ C_{n-\ell+1} & C_{n-\ell+2} \end{vmatrix}}{C_{n-\ell+1}}$$

then $\ell = \ell + 1$.

For $n = \ell-2 \ldots\ldots N-1$,

$$Pg_1(\ell,1-\ell,n;x) = \frac{\begin{vmatrix} x^{\ell-1}q^{n-\ell+1} & x^{\ell}q^{n-\ell}(x) \\ A_{n-\ell+2} & A_{n-\ell+1} \end{vmatrix}}{A_{n-\ell+2}}$$

$$Pg_2(1-\ell,\ell,n;x) = -\frac{\begin{vmatrix} x^{\ell}p^{n-\ell}(x) & x^{\ell-1}p^{n-\ell+1}(x) \\ C_{n-\ell+1} & C_{n-\ell+2} \end{vmatrix}}{C_{n-\ell+2}}$$

Step 5. Set $N = N - 1$.

For $k = 1, 2 \ldots \ell-1$;

If $(\ell-k-2) < 0$ go to Step 6.

a) $Pg_1(\ell, 1-\ell+k, \ell-k-2\,; x) = (-1)^{k+1}\, x^{\ell} q^{-k-2}(x)$

$Pg_2(1-\ell+k, \ell, \ell-k-2\,; x) = -x^{\ell} p^{-k-2}(x)$.

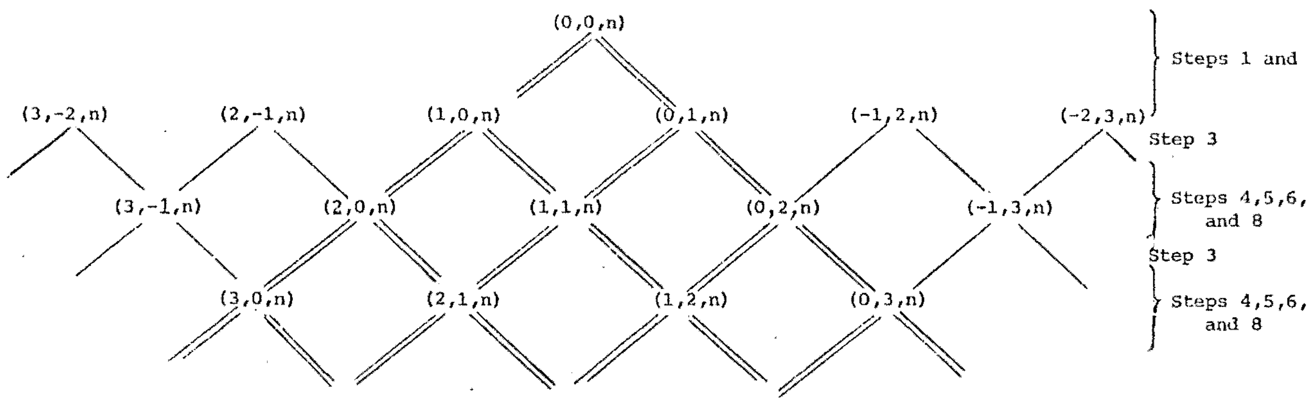
b) For $n = \ell-k-1 \ldots N-1$;

Compute $Pg_1(\ell, 1-\ell+k, n; x)$ by (6.4.2) and

$Pg_2(1-\ell+k, \ell, n; x)$ by (6.4.3).

Steps 6, 7 and 8 same as algorithm I.

The steps can be shown by the following diagram.



Fiugre 6.4.2

Algorithm I involves defining two more arrays $Pg^{n}_{k,j}(x)$ and $Qg^{n}_{k,j}(x)$, but uses less storage and computation. Algorithm II is more generalized but at the cost of larger arrays and double the computation.

<u>Theoretical justification</u>

THEOREM 1 a) *For all integers* $\ell \geqslant 2, m \geqslant 1, n \geqslant 0$.

$$\text{(i)}\quad P(\ell,m,n;x) = \frac{\Delta P(\ell,m-1,n;x)}{\Delta Pg_2(\ell,m,n;x)}\, Pg_2(\ell,m,n;x) - P(\ell,m-1,n;x)$$

$$\text{(ii)}\quad P(\ell,m,n;x) = \frac{\Delta P(\ell-1,m,n;x)}{\Delta Pg_1(\ell,m,n;x)}\, Pg_1(\ell,m,n;x) - P(\ell-1,m,n;x)$$

b) *In addition* (i) *holds for all* P *if* $\ell = 1$, $m \geqslant 1$, $n \geqslant 0$ *and holds for* $P = \beta, \gamma$ if $\ell = 0$, $m \geqslant 1$, $n \geqslant 0$.

(ii) *holds for all* P *if* $\ell \geqslant 2$, $m = 0$, $n \geqslant 0$ *and holds for* $P = \beta, \gamma$ *if* $\ell = 1$, $m \geqslant 0$, $n \geqslant 0$.

Proof: a (i). This can be proved by using the method in [2]. The proof here is similar to that used previously [8].

Using the Sylvester identity to the numerator of $P(\ell,m,n;x)$.

$P(\ell,m,n;x) =$

$$\frac{\begin{vmatrix} x^m p^{n-m}(x) & \cdots & p^n(x) & x^\ell q^{n-\ell}(x) & \cdots & xq^{n-1}(x) \\ C_{n-m+1} & \cdots & C_{n+1} & A_{n-\ell+1} & \cdots & A_n \\ \cdots & & & & & \cdots \\ C_{\ell+n} & \cdots & C_{\ell+m+n} & A_{m+n} & \cdots & A_{\ell+m+n-1} \end{vmatrix}}{\begin{vmatrix} C_{n-m+2} & \cdots & C_{n+1} & A_{n-\ell+1} & \cdots & A_n \\ \cdots & & & & & \cdots \\ C_{\ell+n+1} & \cdots & C_{\ell+m+n} & A_{m+n} & \cdots & A_{\ell+m+n-1} \end{vmatrix}} \cdot \frac{\begin{vmatrix} C_{n-m+2} & \cdots & C_{n+1} & A_{n-\ell+1} & \cdots & A_{n+1} \\ \cdots & & & & & \cdots \\ C_{\ell+n+2} & \cdots & C_{\ell+m+n+1} & A_{m+n+1} & \cdots & A_{\ell+m+n+1} \end{vmatrix}}{\begin{vmatrix} C_{n-m+1} & & C_{n+1} & A_{n-\ell+1} & \cdots & A_n \\ \cdots & & & & & \cdots \\ C_{\ell+n+1} & \cdots & C_{\ell+m+n+1} & A_{m+n+1} & \cdots & A_{\ell+m+n} \end{vmatrix}}$$

$$- \frac{\begin{vmatrix} x^{m-1} p^{n-m+1}(x) & \cdots & p^n(x) & x^\ell q^{n-\ell}(x) & \cdots & q^n(x) \\ C_{n-m+2} & \cdots & C_{n+1} & A_{n-\ell+1} & \cdots & A_{n+1} \\ \cdots & & & & & \cdots \\ C_{\ell+n+1} & \cdots & C_{\ell+m+n} & A_{m+n} & \cdots & A_{\ell+m+n} \end{vmatrix}}{\begin{vmatrix} C_{n-m+2} & \cdots & C_{n+1} & A_{n-\ell+1} & \cdots & A_n \\ \cdots & & & & & \cdots \\ C_{\ell+n+1} & \cdots & C_{\ell+m+n} & A_{m+n} & \cdots & A_{\ell+m+n-1} \end{vmatrix}}$$

The second term of the right hand side is exactly $P(\ell,m-1,n;x)$. We define the first factor of the first term as $-Pq_2(\ell,m,n;x)$. The second factor of the first term can be shown to be the ratio of the forward differences of the index n of $P(\ell,m-1,n;x)$ and $Pq_2(\ell,m,n;x)$. Since $P(\ell,m-1,n;x)$ and $Pq_2(\ell,m,n;x)$ both have the same denominator, by cross multiplying, we have

$$\frac{\Delta P(\ell,m-1,n;x)}{\Delta Pg_2(\ell,m,n;x)} = (-1)^{\ell+m} \times$$

$$\left\{ \begin{vmatrix} x^{m-1}p^{n-m+2}(x) & \cdots & p^{n+1}(x) & x^{\ell}q^{n-\ell+1}(x) & \cdots & q^{n+1}(x) \\ C_{n-m+3} & \cdots & C_{n+2} & A_{n-\ell+2} & \cdots & A_{n+2} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ C_{\ell+n+2} & \cdots & C_{\ell+m+n+1} & A_{m+n+1} & \cdots & A_{\ell+m+n+1} \end{vmatrix} \begin{vmatrix} 1 & x^{m-1}p^{n-m+1}(x) & \cdots & p^{n}(x) & x^{\ell}q^{n-\ell}(x) & \cdots & xq^{n-1}(x) \\ 0 & C_{n-m+2} & \cdots & C_{n+1} & A_{n-\ell+1} & \cdots & A_{n} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & C_{\ell+n+1} & \cdots & C_{\ell+m+n} & A_{m+n} & \cdots & A_{\ell+m+n-1} \end{vmatrix} \right.$$

$$\left. - \begin{vmatrix} x^{m-1}p^{n+m+1}(x) & \cdots & p^{n}(x) & x^{\ell}q^{n-\ell}(x) & \cdots & q^{n}(x) \\ C_{n-m+2} & \cdots & C_{n+1} & A_{n-\ell+1} & \cdots & A_{n+1} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ C_{\ell+n+1} & \cdots & C_{\ell+m+n} & A_{m+n} & \cdots & A_{\ell+m+n} \end{vmatrix} \begin{vmatrix} 1 & x^{m-1}p^{n-m+2}(x) & \cdots & p^{n+1}(x) & x^{\ell}q^{n-\ell+1}(x) & \cdots & xq^{n}(x) \\ 0 & C_{n-m+3} & \cdots & C_{n+2} & A_{n-\ell+2} & \cdots & A_{n+1} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & C_{\ell+n+2} & \cdots & C_{\ell+m+n+1} & A_{m+n+1} & \cdots & A_{\ell+m+n} \end{vmatrix} \right\} \Big/$$

$$- \left\{ \begin{vmatrix} x^{m}p^{n-m+1}(x) & \cdots & p^{n+1}(x) & x^{\ell}q^{n-\ell+1}(x) & \cdots & xq^{n}(x) \\ C_{n-m+2} & \cdots & C_{n+2} & A_{n-\ell+2} & \cdots & A_{n+1} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ C_{\ell+n+1} & \cdots & C_{\ell+m+n+1} & A_{m+n+1} & \cdots & A_{\ell+m+n} \end{vmatrix} \begin{vmatrix} x^{m-1}p^{n-m+1}(x) & \cdots & p^{n}(x) & x^{\ell}q^{n-\ell}(x) & \cdots & xq^{n-1}(x) & 1 \\ C_{n-m+2} & \cdots & C_{n+1} & A_{n-\ell+1} & \cdots & A_{n} & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ C_{\ell+n+1} & \cdots & C_{\ell+m+n} & A_{m+n} & \cdots & A_{\ell+m+n-1} & 0 \end{vmatrix} \right.$$

$$\left. - \begin{vmatrix} x^{m}p^{n-m}(x) & \cdots & p^{n}(x) & x^{\ell}q^{n-\ell}(x) & \cdots & xq^{n-1}(x) \\ C_{n-m+1} & \cdots & C_{n+1} & A_{n-\ell+1} & \cdots & A_{n} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ C_{\ell+n} & \cdots & C_{\ell+m+n} & A_{m+n} & \cdots & A_{\ell+m+n-1} \end{vmatrix} \begin{vmatrix} x^{m-1}p^{n-m+2}(x) & \cdots & p^{n+1}(x) & x^{\ell}q^{n-\ell+1}(x) & \cdots & xq^{n}(x) & 1 \\ C_{n-m+3} & \cdots & C_{n+2} & A_{n-\ell+2} & \cdots & A_{n+1} & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ C_{\ell+n+2} & \cdots & C_{\ell+m+n+1} & A_{m+n+1} & \cdots & A_{\ell+m+n} & 0 \end{vmatrix} \right\}$$

After some row operation and using Sylvester's identity, it follows

$$\frac{\Delta P(\ell,m-1,n;x)}{\Delta Pg_2(\ell,m,n;x)} = (-1)^{\ell+m} \frac{\begin{vmatrix} 0 & C_{n-m+2} & \cdots & C_{n+1} & A_{n-\ell+1} & \cdots & A_{n+1} \\ 1 & x^{m-1}p^{n-m+2}(x) & \cdots & p^{n+1}(x) & x^{\ell}q^{n-\ell+1}(x) & \cdots & q^{n+1}(x) \\ 0 & C_{n-m+3} & \cdots & C_{n+2} & A_{n-\ell+2} & \cdots & A_{n+2} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & C_{\ell+n+2} & \cdots & C_{\ell+m+n+1} & A_{m+n+1} & \cdots & A_{\ell+m+n+1} \end{vmatrix}}{\begin{vmatrix} C_{n-m+1} & \cdots & C_{n+1} & A_{n-\ell+1} & \cdots & A_{n} & 0 \\ x^{m}p^{n-m+1}(x) & \cdots & p^{n+1}(x) & x^{\ell}q^{n-\ell+1}(x) & \cdots & xq^{n}(x) & 1 \\ C_{n-m+2} & \cdots & C_{n+2} & A_{n-\ell+2} & \cdots & A_{n+1} & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ C_{\ell+n+1} & \cdots & C_{\ell+m+n+1} & A_{m+n+1} & \cdots & A_{\ell+m+n} & 0 \end{vmatrix}}$$

$$\frac{\begin{vmatrix} C_{n-m+2} & \cdots & C_{n+1} & A_{n-\ell+1} & \cdots & A_{n+1} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ C_{\ell+n+2} & \cdots & C_{\ell+m+n+1} & A_{m+n+1} & \cdots & A_{\ell+m+n+1} \end{vmatrix}}{\begin{vmatrix} C_{n-m+1} & \cdots & C_{n+1} & A_{n-\ell+1} & \cdots & A_{n} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ C_{\ell+n+1} & \cdots & C_{\ell+m+n+1} & A_{m+n+1} & \cdots & A_{\ell+m+n} \end{vmatrix}} \qquad (6.4.6)$$

a(ii) Shift the (m+2) th column of (6.2.2) to the first column and use the same method as in a(i).

$$P(\ell,m,n;x) =$$

$$\frac{\begin{vmatrix} x^{\ell}q^{n-\ell}(x) & x^{m}p^{n-m}(x) & \cdots & p^{n}(x) & x^{\ell-1}q^{n-\ell+1}(x) & \cdots & xq^{n-1}(x) \\ A_{n-\ell+1} & C_{n-m+1} & \cdots & C_{n+1} & A_{n-\ell+2} & \cdots & A_{n} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ A_{m+n} & C_{\ell+n} & \cdots & C_{\ell+m+n} & A_{m+n+1} & \cdots & A_{\ell+m+n-1} \end{vmatrix} \begin{vmatrix} C_{n-m+1} & \cdots & C_{n+1} & A_{n-\ell+2} & \cdots & A_{n+1} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ C_{\ell+n+1} & \cdots & C_{\ell+m+n+1} & A_{m+n+2} & \cdots & A_{\ell+m+n+1} \end{vmatrix}}{\begin{vmatrix} C_{n+m+1} & \cdots & C_{n+1} & A_{n-\ell+2} & \cdots & A_{n} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ C_{\ell+n} & \cdots & C_{\ell+m+n} & A_{m+n+1} & \cdots & A_{\ell+m+n-1} \end{vmatrix} \begin{vmatrix} C_{n-m+1} & \cdots & C_{n+1} & A_{n-\ell+2} & \cdots & A_{n} & A_{n-\ell+1} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ C_{\ell+n+1} & \cdots & C_{\ell+m+n-1} & A_{m+n+2} & \cdots & A_{\ell+m+n} & A_{m+n+1} \end{vmatrix}}$$

$$- \frac{\begin{vmatrix} x^{m}p^{n-m}(x) & \cdots & p^{n}(x) & x^{\ell-1}q^{n-\ell+1}(x) & \cdots & q^{n}(x) \\ C_{n-m+1} & \cdots & C_{n+1} & A_{n-\ell+2} & \cdots & A_{n+1} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ C_{\ell+n} & \cdots & C_{\ell+m+n} & A_{m+n+1} & \cdots & A_{\ell+m+n} \end{vmatrix}}{\begin{vmatrix} C_{n-m+1} & \cdots & C_{n+1} & A_{n-\ell+2} & \cdots & A_{n} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ C_{\ell+n} & \cdots & C_{\ell+m+n} & A_{m+n+1} & \cdots & A_{\ell+m+n-1} \end{vmatrix}}$$

The second term of the right hand side is exactly $P(\ell-1,m,n;x)$. In order to be symmetric with $Pg_2(\ell,m,n;x)$. Shift the first column of the first factor of the first term to the last column and then define the first factor of the first term as $Pg_1(\ell,m,n;x)$. The second factor of the first term can be shown to be the ratio of the differences on the index n of $P(\ell-1,m,n;x)$ and $Pg_1(\ell,m,n;x)$ by the same method as in a(i). We have

$$\frac{\Delta P(\ell-1,m,n;x)}{\Delta Pq_1(\ell,m,n;x)} =$$

$$\left\{ \begin{vmatrix} x^m p^{n-m+1}(x) & \cdots & p^{n+1}(x) & x^{\ell-1}q^{n-\ell+2}(x) & \cdots & q^{n+1}(x) \\ C_{n-m+2} & \cdots & C_{n+2} & A_{n-\ell+3} & \cdots & A_{n+2} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ C_{\ell+n+1} & \cdots & C_{\ell+m+n+1} & A_{m+n+2} & \cdots & A_{\ell+m+n+1} \end{vmatrix} \begin{vmatrix} 1 & x^m p^{n-m}(x) & \cdots & p^{n+1}(x) & x^{\ell-1}q^{n-\ell+1}(x) & \cdots & xq^n(x) \\ 0 & C_{n-m+1} & \cdots & C_{n+1} & A_{n-\ell+2} & \cdots & A_n \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & C_{\ell+n} & \cdots & C_{\ell+m+n} & A_{m+n+1} & \cdots & A_{\ell+m+n-1} \end{vmatrix} \right.$$

$$\left. - \begin{vmatrix} x^m p^{n-m}(x) & \cdots & p^n(x) & x^{\ell-1}q^{n-\ell+1}(x) & \cdots & q^n(x) \\ C_{n-m+1} & \cdots & C_{n+1} & A_{n-\ell+2} & \cdots & A_{n+1} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ C_{\ell+n} & \cdots & C_{\ell+m+n} & A_{m+n+1} & \cdots & A_{\ell+m+n} \end{vmatrix} \begin{vmatrix} 1 & x^m p^{n-m+1}(x) & \cdots & p^{n+1}(x) & x^{\ell-1}q^{n-\ell+2}(x) & \cdots & q^{m+1}(x) \\ 0 & C_{n-m+2} & \cdots & C_{n+2} & A_{n-\ell+3} & \cdots & A_{n+1} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & C_{\ell+n+1} & \cdots & C_{\ell+m+n+1} & A_{m+n+2} & \cdots & A_{\ell+m+n} \end{vmatrix} \right\} \Big/$$

$$\left\{ \begin{vmatrix} x^m p^{n-m+1}(x) & \cdots & p^{n+1}(x) & x^{\ell-1}q^{n-\ell+2}(x) & \cdots & xq^n(x) & x^{\ell}q^{n-\ell+1}(x) \\ C_{n-m+2} & \cdots & C_{n+2} & A_{n-\ell+3} & \cdots & A_{n+1} & A_{n-\ell+2} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ C_{\ell+n+1} & \cdots & C_{\ell+m+n+1} & A_{m+n+2} & \cdots & A_{\ell+m+n} & A_{m+n+1} \end{vmatrix} \begin{vmatrix} 1 & x^m p^{n-m}(x) & \cdots & p^n(x) & x^{\ell-1}q^{n-\ell+1}(x) & \cdots & xq^{n-1}(x) \\ 0 & C_{n-m+1} & \cdots & C_{n+1} & A_{n-\ell+2} & \cdots & A_n \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & C_{\ell+n} & \cdots & C_{\ell+m+n} & A_{m+n+1} & \cdots & A_{\ell+m+n-1} \end{vmatrix} \right.$$

$$\left. - \begin{vmatrix} x^m p^{n-m}(x) & \cdots & p^n(x) & x^{\ell+1}q^{n-\ell+1}(x) & \cdots & xq^{n-1}(x) & x^{\ell}q^{n-\ell}(x) \\ C_{n-m+1} & \cdots & C_{n+1} & A_{n-\ell+2} & \cdots & A_n & A_{n-\ell+1} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ C_{\ell+n} & \cdots & C_{\ell+m+n} & A_{m+n+1} & \cdots & A_{\ell+m+n-1} & A_{m+n} \end{vmatrix} \begin{vmatrix} 1 & x^m p^{n-m+1}(x) & \cdots & p^{n+1}(x) & x^{\ell-1}q^{n-\ell+2}(x) & \cdots & xq^n(x) \\ 0 & C_{n-m+2} & \cdots & C_{n+2} & A_{n-\ell+3} & \cdots & A_{n+1} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & C_{\ell+n+1} & \cdots & C_{\ell+m+n+1} & A_{m+n+2} & \cdots & A_{\ell+m+n} \end{vmatrix} \right\}$$

$$
= \frac{\begin{vmatrix} 0 & C_{n-m+1} & \cdots & C_{n+1} & A_{n-\ell+2} & \cdots & A_{n+1} \\ 1 & x^m p^{n-m+1}(x) & \cdots & p^{n+1}(x) & q^{n-\ell+2}(x) & \cdots & q^{n+1}(x) \\ 0 & C_{n-m+2} & \cdots & C_{n+2} & A_{n-\ell+3} & \cdots & A_{n+2} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & C_{\ell+n+1} & \cdots & C_{\ell+m+n+1} & A_{m+n+2} & \cdots & A_{\ell+m+n+1} \end{vmatrix}}{\begin{vmatrix} 0 & C_{n-m+1} & \cdots & C_{n+1} & A_{n-\ell+2} & \cdots & A_{n} & A_{n-\ell+1} \\ 1 & x^m p^{n-m+1}(x) & \cdots & p^{n+1}(x) & x^{\ell-1} q^{n-\ell+2}(x) & \cdots & x q^{n}(x) & x^{\ell} q^{n-\ell+1}(x) \\ 0 & C_{n-m+2} & \cdots & C_{n+2} & A_{n-\ell+3} & \cdots & A_{n+1} & A_{n-\ell+2} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & C_{\ell+n+1} & \cdots & C_{\ell+m+n+1} & A_{m+n+2} & \cdots & A_{\ell+m+n} & A_{m+n+1} \end{vmatrix}}
$$

$$
= \frac{\begin{vmatrix} C_{n-m+1} & \cdots & C_{n+1} & A_{n-\ell+2} & \cdots & A_{n+1} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ C_{\ell+n+1} & \cdots & C_{\ell+m+n+1} & A_{m+n+2} & \cdots & A_{\ell+m+n+1} \end{vmatrix}}{\begin{vmatrix} C_{n-m+1} & \cdots & C_{n+1} & A_{n-\ell+2} & \cdots & A_{n} & A_{n-\ell+1} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ C_{\ell+n+1} & \cdots & C_{\ell+m+n+1} & A_{m+n+2} & \cdots & A_{\ell+m+n} & A_{m+n+1} \end{vmatrix}} \qquad (6.4.7)
$$

b(i) If $\ell=1$, then the proof of a(i) still holds.

If $\ell=0$ the proof breaks down in the case $P=\alpha$, since $\alpha g_2(0,m,n;x) = 0 \ \forall n$. However the imposed normalization condition implies that $\alpha(0,m,n;x) = 1$ and hence these values do not need to be calculated.

b(ii) If $m=0$ then the proof of a(ii) still holds. If $\ell=1$ the proof breaks down in the case $P=\alpha$, since $\alpha g_1(1,m,n;x) = (-1)^{m+1}x$ for $m \geqslant 0$, $n \geqslant 0$ and hence $\Delta\alpha g_1(1,m,n;x) = 0$. However as noted above in b(i), $\alpha(0,m,n;x) = 1$ and hence $\Delta\alpha(0,m,n;x) = 0$. Thus the ratio $\Delta\alpha(0,m,n;x)/\Delta\alpha g_1(1,m,n;x)$ is not defined. It is clear from (6.4.7) that this ratio does have a definite value and the decomposition is still true but its expression in terms of the differences for the computational algorithm cannot be used.

Note 1. The expressions for $Pg_1(\ell,m,n;x)$ and $-Pg_2(\ell,m,n;x)$ have common numerators and the denominators have one column different. The denominator of $Pg_1(\ell,m,n;x)$ has one more column of C's and one less column of A's than $pg_2(\ell,m,n;x)$.

2. The expressions for $Pg_1(\ell-1,m,n;x)$ and $-Pg_2(\ell-1,m,n;x)$ have the same denominators but the numerators have one column different. The numberator of $Pg_1(\ell,m-1,n;x)$ has one more column of A's and one less column of C's than $Pg_2(\ell-1,m,n;x)$.

3. The ratios (6.4.6) and (6.4.7) are constants and each has the same ratio for $P=\alpha,\beta$ and γ (See Corollary 4). They

can be expressed as the ratios of $\Delta P(\ell-1,m,n;x)/\Delta Pg_1(\ell,m,n;x)$ and $\Delta P(\ell,m-1,n;x)/\Delta Pg_2(\ell,m,n;x)$ for convenience in computation, but in some cases, such as Theorem 1(b), these ratios cannot be expressed in terms of differences of the respective P. However, since p(x) and q(x) are different from zero in the case $P = \gamma$, if the ratios are expressed in terms of the respective γ and γg_i, the algorithm will not break down.

$Qg_{\ell,j}^{\,n}(x)$ in algorithm I can be expressed

$$\frac{\begin{vmatrix} x^{\ell-1}q^{n-\ell+1}(x) & \cdots & xq^{n-1}(x) & p^n(x) & x^{j-1}q^{n-j+1}(x) \\ A_{n-\ell+2} & \cdots & A_n & C_{n+1} & A_{n-j+2} \\ A_{n+1} & \cdots & A_{\ell+n-1} & C_{\ell+n} & A_{n-j+\ell+1} \end{vmatrix}}{\begin{vmatrix} A_{n-\ell+2} & \cdots & A_n & C_{n+1} \\ \cdots & \cdots & \cdots & \cdots \\ A_{n+1} & \cdots & A_{\ell+n-1} & C_{\ell+n} \end{vmatrix}}$$

and $Pg_{\ell,j}^{\,n}(x)$ can be expressed as

$$\frac{\begin{vmatrix} x^{j-1}p^{n-j+1}(x) & x^{\ell-1}p^{n-\ell+1}(x) & \cdots & xp^{n-1}(x) & p^n(x) \\ C_{n-j+2} & C_{n-\ell+2} & \cdots & C_n & C_{n+1} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ C_{n-j+\ell+1} & C_{n+1} & \cdots & C_{\ell+n-1} & C_{\ell+n} \end{vmatrix}}{\begin{vmatrix} C_{n-\ell+2} & \cdots & C_{n+1} \\ \cdots & \cdots & \cdots \\ C_{n+1} & \cdots & C_{\ell+n} \end{vmatrix}}$$

COROLLARY 1. *For all integers* $\ell \geqslant 2,\ n \geqslant 0$

$$Qg_{\ell,j}^{\ n}(x) = \frac{\Delta Qg_{\ell-1,j}^{\ n}(x)}{\Delta Qg_{\ell-1,\ell}^{\ n}(x)}\ Qg_{\ell-1,\ell}^{\ n}(x) - Qg_{\ell-1,j}(x) \quad \textit{where} \quad j = \ell+1, \ell+2 \ldots$$

holds for all $Q = \alpha, \beta$ and γ.

Proof : Same as Theorem 1.

COROLLARY 2. *For all integers* $\ell \geqslant 2,\ n \geqslant 0$

$$Pg_{\ell,j}^{\ n}(x) = \frac{\Delta Pg_{\ell-1,j}^{\ n}(x)}{\Delta Pg_{\ell-1,\ell}^{\ n}(x)}\ Pg_{\ell-1,\ell}^{\ n}(x) - Pg_{\ell-1,j}^{\ n}(x) \quad \textit{where} \quad j = \ell+1,\ \ell+2 \ldots$$

holds for all $P = \beta$ and γ .

(Note $\alpha g_{\ell,j}^{\ n}(x) = 0 \ \forall\, n.$)

Proof : Same as Theorem 1.

In the case of negative arguments $Pg_i(\ell,-j,n;x)$ can be expressed as follows:

$$Pg_1(\ell,-j,n;x) = \frac{\begin{vmatrix} x^{\ell-1}q^{n-\ell+1} & \cdots & x^j q^{n-j}(x) & x^{\ell} q^{n-\ell}(x) \\ A_{n-\ell+2} & \cdots & A_{n-j+1} & A_{n-\ell+1} \\ A_{n-j+1} & \cdots & A_{\ell+n-2j} & A_{n-j} \end{vmatrix}}{\begin{vmatrix} A_{n-\ell+2} & \cdots & A_{n-j+1} \\ \cdot & \cdots & \cdot \\ A_{n-j+1} & \cdots & A_{\ell+n-2j} \end{vmatrix}} \qquad n \geqslant j-1$$

$$Pg_2(\ell,-j,n;x) = -\frac{\begin{vmatrix} x^j q^{n-j}(x) & x^{j+1}q^{n-j-1}(x) & \cdots & x^\ell q^{n-\ell}(x) \\ A_{n-j+1} & A_{n-j} & \cdots & A_{n-\ell+1} \\ \cdots & \cdots & \cdots & \cdots \\ A_{\ell+n-2j} & A_{\ell+n-2j-1} & \cdots & A_{n-j} \end{vmatrix}}{\begin{vmatrix} A_{n-j} & \cdots & A_{n-\ell+1} \\ \cdots & \cdots & \cdots \\ A_{\ell+n-2j-1} & \cdots & A_{n-j} \end{vmatrix}} \qquad n \geqslant j$$

where $j = 1,2....$

$$Pg_1(\ell,0,n;x) = \frac{\begin{vmatrix} x^{\ell-1}q^{n-\ell+1}(x) & \cdots & xq^{n-1}(x) & p^n(x) & x^\ell q^{n-\ell}(x) \\ A_{n-\ell+2} & \cdots & A_n & C_{n+1} & A_{n-\ell+1} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ A_{n+1} & \cdots & A_{\ell+n-1} & C_{\ell+n} & A_n \end{vmatrix}}{\begin{vmatrix} A_{n-\ell+2} & \cdots & A_n & C_{n+1} \\ \cdots & \cdots & \cdots & \cdots \\ A_{n+1} & \cdots & A_{\ell+n-1} & C_{\ell+n} \end{vmatrix}}$$

which has the same expression as $Qg^n_{\ell,\ell+1}(x)$

$$Pg_2(\ell,0,n;x) = -\frac{\begin{vmatrix} p^n(x) & x^\ell q^{n-\ell}(x) & \cdots & xq^{n-1}(x) \\ C_{n+1} & A_{n-\ell+1} & \cdots & A_n \\ \cdots & \cdots & \cdots & \cdots \\ C_{\ell+m+n} & A_{m+n} & \cdots & A_{\ell+m+n-1} \end{vmatrix}}{\begin{vmatrix} A_{n-\ell+1} & \cdots & A_n \\ \cdots & \cdots & \cdots \\ A_{m+n} & \cdots & A_{\ell+m+n-1} \end{vmatrix}}$$

which is the same expression as $Pg^n_{\ell,\ell+1}(x)$

$$Pg_1(-j,m,n;x) = \frac{\begin{vmatrix} x^m p^{n-m}(x) & \cdots & x^j p^{n-j}(x) \\ C_{n-m+1} & \cdots & C_{n-j+1} \\ \cdots & \cdots & \cdots \\ C_{n-j} & \cdots & C_{m+n-2j} \end{vmatrix}}{\begin{vmatrix} C_{n-m+1} & \cdots & C_{n-j} \\ C_{n-j} & \cdots & C_{m+n-2j-1} \end{vmatrix}} \qquad n \geqslant j$$

$$Pg_2(-j,m,n;x) = \frac{\begin{vmatrix} x^m p^{n-m}(x) & \cdots & x^j p^{n-j}(x) \\ C_{n-m+1} & \cdots & C_{n-j+1} \\ \cdots & \cdots & \cdots \\ C_{n-j} & \cdots & C_{m+n-2j} \end{vmatrix}}{\begin{vmatrix} C_{n-m+2} & \cdots & C_{n-j+1} \\ \cdots & \cdots & \cdots \\ C_{n-j+1} & \cdots & C_{m+n-2j} \end{vmatrix}} \qquad n \geqslant j-1$$

where $j = 0,1,2\ldots$

COROLLARY 3

(a) *For all integers* $\ell,m,n \geqslant 0$ *and* $\ell + m \neq 1$

(i) $$Pg_1(\ell,m,n;x) = \frac{\Delta Pg_1(\ell,m-1,n;x)}{\Delta Pg_2(\ell-1,m,n;x)} \quad Pg_2(\ell-1,m,n;x) - Pg_1(\ell,m-1,n;x)$$

(ii) $$Pg_2(\ell,m,n;x) = \frac{\Delta Pg_2(\ell-1,m,n;x)}{\Delta Pg_1(\ell,m-1,n;x)} \quad Pg_1(\ell,m-1,n;x) - Pg_2(\ell-1,m,n;x)$$

(b) *For* $\ell > 2$, $m < 0$ *and* $\ell + m \neq 1$, $n \geqslant |m|$ (i) *and* (ii) *hold*.

(c) *For* $m > 2$, $\ell < 0$ *and* $\ell + m \neq 1$, $n \geqslant |\ell|$ (i) *and* (ii) *hold.*

Proof : Similar to Theorem 1.

Note : 1. For the computation of $Pg_i(\ell,-j,n;x)$ and $Pg_i(-j,m,n;x)$ on the index n, in algorithm II, n increases from j. For $n < j$, $Pg_2(\ell,-j,n;x)$ and $Pg_1(-j,m,n;x)$ do not exist and for $n < j-1$, $Pg_1(\ell,-j,n;x)$ and $Pg_2(-j,m,n;x)$ do not exist. Although $Pg_1(\ell,-j,j-1;x)$ and $Pg_2(-j,m,j-1;x)$ cannot be computed by the algorithm (since $Pg_2(\ell-1,-j,j-1;x)$, $Pg_1(\ell,-j-1,j-1;x)$, $Pg_1(-j,m-1,j-1;x)$ and $Pg_2(-j-1,m,j-1;x)$ do not exist) the previously defined expressions for $Pg_1(\ell,-j,n;x)$ and $Pg_2(-j,m,n;x)$ reduce to a single term in the case n=j-1. Hence they can be defined (or initialized) in the algorithm as

$$Pg_1(\ell,-j,j-1;x) = (-1)^{\ell-j} x^{\ell} q^{j-\ell-1}(x)$$

and

$$Pg_2(-j,m,j-1\,x) = -\,x^m p^{j-m-1}(x)\ .$$

2. The '-' sign in $Pg_2(\ell,m,n;x)$ is designed to unify (6.4.2) and (6.4.3). If the '-' is omitted, (6.4.2) will be

$$Pg_2(\ell,m,n;x) = Pg_2(\ell-1,m,n;x) - \frac{\Delta\gamma g_2(\ell-1,m,n;x)}{\Delta\gamma g_1(\ell,m-1,n;x)}\, Pg_1(\ell,m-1,n;x)$$

<u>COROLLARY 4</u>

$$\frac{\Delta P(\ell-1,m,n;x)}{\Delta Pg_1(\ell,m,n;x)}\ ,\quad \frac{\Delta P(\ell,m-1,n;x)}{\Delta Pg_2(\ell,m,n;x)}\ ,\quad \frac{\Delta Pg_1(\ell,m-1,n;x)}{\Delta Pg_2(\ell-1,m,n;x)}$$

and $\dfrac{\Delta Pg_2(\ell-1,m,n;x)}{\Delta Pg_1(\ell,m-1,n;x)}$ *are defined they are constants and each one has same ratio for* $P = \alpha,\beta$ *and* γ.

Proof : The first and second ratios have been shown to be constant in (6.4.6) and (6.4.7). The other two ratios are also constant by a smilar method.

6.5 ACCELERATION OF THE CONVERGENCE OF SEQUENCES

It is well known that the epsilon algorithm gives a recursive procedure when evaluating a Pade approximant at a point $x = 1$. This is used in the acceleration of the convergence of a sequence. The quadratic approximation can be similarly applied.

Let $S(x) = S_0 + \sum_{i=1}^{\infty} \Delta S_{i-1} x^i$ for a sequence $\{S_n = 0,1\ldots\}$

Then the partial sum $S_n(x)$ of $S(x)$ is

$$S_n(x) = S_0 + \sum_{i=1}^{n} \Delta S_{i-1} x^i$$

where $S_n(1) = S_n$

$$\Delta S_i = S_{i+1} - S_i \quad .$$

Let $T(x)$ be the square of $S(x)$, then the partial sum $T_n(x)$ of $T(x)$ is $T_n(x) = T_0 + \sum_{i=1}^{n} \Delta T_{i-1} x^i$

where $T_n(1) = T_n$

$$\Delta T_i = T_{i+1} - T_i \quad .$$

Now if $\{S_n\}$ is extrapolated by quadratic approximation, then from (6.2.2) we have

$$P(\ell,m,n;1) = \frac{\begin{vmatrix} p^{n-m}(1) & \cdot\cdot & p^{n}(1) & q^{n-\ell}(1) & \cdot\cdot & q^{n}(1) \\ \Delta S_{n-m} & \cdot\cdot & \Delta S_{n} & \Delta T_{n-\ell} & \cdot\cdot & \Delta T_{n} \\ \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot & \cdot\cdot \\ \Delta S_{\ell+n} & \cdot\cdot & \Delta S_{\ell+m+n} & \Delta T_{n+m} & \cdot\cdot & \Delta T_{\ell+m+n} \end{vmatrix}}{D}$$

where for
$$\left.\begin{array}{lll} P = \alpha; & p^i(1) = 0, & q^i(1) = 1 \\ P = \beta; & p^i(1) = 1 & q^i(1) = 0 \end{array}\right\} \forall i$$
$$P = \gamma; \quad p^i(1) = -S_i \quad q^i(1) = -T_i \quad i = 0,1,2\ldots$$

where $C_{i+1} = \Delta S_i$, $A_{i+1} = \Delta T_i$

and $S_i = 0$, $T_i = 0$ if $i < 0$.

The quadratic function with coefficients $P(\ell,m,n;1)$ is considered and the root closest to the previous approximation as the extrapolated value of the sequence $\{S_n\}$ is taken. This process essentially generalizes Wynn's ε-algorithm which uses a rational rather than a quadratic approximation.

The extrapolation algorithm is simialr to the algorithm described in Section 6.4 and it is the extension of ε-algorithm [3] except for a small change in the initialization.

For convenience $P(\ell,m,n;1) = P(\ell,m,n)$, $Pg_i(\ell,m,n;1) = Pg_i(\ell,m,n)$ and $Pg_{k,j}^n(x) = Pg_{k,j}^n$.

Algorithm III.

Step 1. For $n = 0,1\ldots.N$,

initialize $Qg_{0,1}^n = Pg_{0,1}^n = p^n$

$$Qg_{0,2}^n = q^{n-1}$$

$$Pg_{0,2}^n = p^{n-1} .$$

Step 2. Set $\ell = 1$,

For $n = 0,1\ldots N-1$;

Compute $P(0,0,n) = \dfrac{\Delta T_n}{\Delta S_n} p^n - q^n$.

Compute $Qg_{1,2}^n$ and $Pg_{1,2}^n$ by (6.4.1);

define $Pg_1(1,0,n) = Qg_{1,2}^n$

$$Pg_2(0,1,n) = Pg_{1,2}^n .$$

Step 3. For $n = 0,1...N-2$;

Compute $P(1,0,n)$ by (6.4.4) and $P(0,1,n)$ by (6.4.5).

Define $NT = N$.

Step 4. Termination criterion.

If $\ell = NT - 2$ stop.

$\ell = \ell + 1$ otherwise.

Step 5. Set $N = NT$.

$j = \ell + 1$;

For $n = 1....N$,

initialize
$$Qg_{0,j}^{n} = q^{n-j+1}$$
$$Pg_{0,j}^{n} = p^{n-j+1} .$$

Step 6. Set $N = N - 1$.

For $k = 1...\ell$;

$n = 0,1...N-1$;

Compute $Qg_{k,j}^{n}$ and $Pg_{k,j}^{n}$ by (4.1),

then define
$$Pg_1(\ell,0,n) = Qg_{\ell,\ell+1}^{n}(x)$$
$$Pg_2(0,\ell,n) = Pg_{\ell,\ell+1}^{n}(x) .$$

Steps 7, 8 and 9 are the same as steps 6, 7 and 8 in algorithm I. Go to step 4.

For extrapolation, the $Pg_{k,j}^{n}$ array is started from $Pg_{0,j}^{n}$. It is shown by the following diagram (figure 6.5.1).

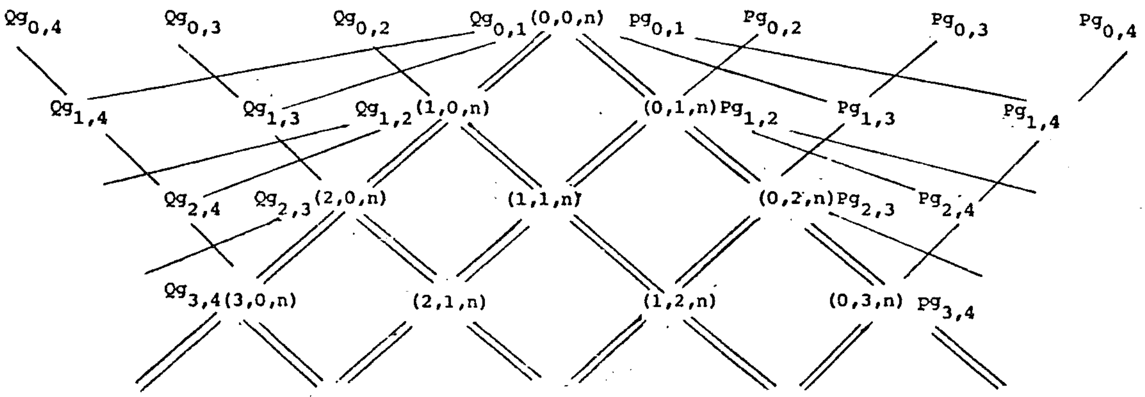


Figure 6.5.1

Algorithm IV

Step 1. For $n = 0,1 \ldots N$,

initialize $Pg_1(0,0,n) = Pg_2(0,0,n) = p^n$

$Pg_2(1,-1,n) = q^{n-1}$

$Pg_1(-1,1,n) = p^{n-1}$.

Step 2. Set $\ell = 1$.

For $n = 0,1 \ldots N-1$;

Compute $P(0,0,n) = \dfrac{\Delta T_n}{\Delta S_n} p^n - q^n$.

Compute $Pg_1(1,0,n)$ from (6.4.2)

and $Pg_2(0,1,n)$ from (6.4.3).

Step 3. Same as step 3 in algorithm III.

Step 4. Termination criterion.

If $\ell = NT - 2$ stop.

Step 5. Set N = NT.

For $n = \ell-1......N-1$,

initialize $Pg_2(\ell,-\ell,n;x) = q^{n-\ell+1}$

$pg_1(-\ell,\ell,n;x) = p^{n-\ell+1}$

then $\ell = \ell + 1$.

For $n = \ell - 2...N-1$

$Pg_1(\ell,-\ell,n) = q^{n-\ell+1}$

$Pg_2(-\ell,\ell,n) = p^{n-\ell+1}$.

Step 6. Set N = N-1.

For $k = 0,1...\ell-1$;

If $(\ell-k-2) < 0$ go to (b).

a). $Pg_1(\ell,1-\ell+k, \ell-k-2) = (-1)^{k+1} q^{-k-2}$

$Pg_2(1-\ell+k,\ell,\ell-k-2) = - p^{-k-2}$

b). For $n = \ell-k-1,....N-1$;

Compute $Pg_1(\ell,1-\ell+k,n)$ by (6.4.2) and $Pg_2(1-\ell+k,\ell,n)$ by (6.4.3).

Steps 7,8 and 9 are the same as steps 7,8 and 9 in algorithm I. The $Pg_i(\ell,m,n)$ array is shown by the following diagram (figure 6.5.2).

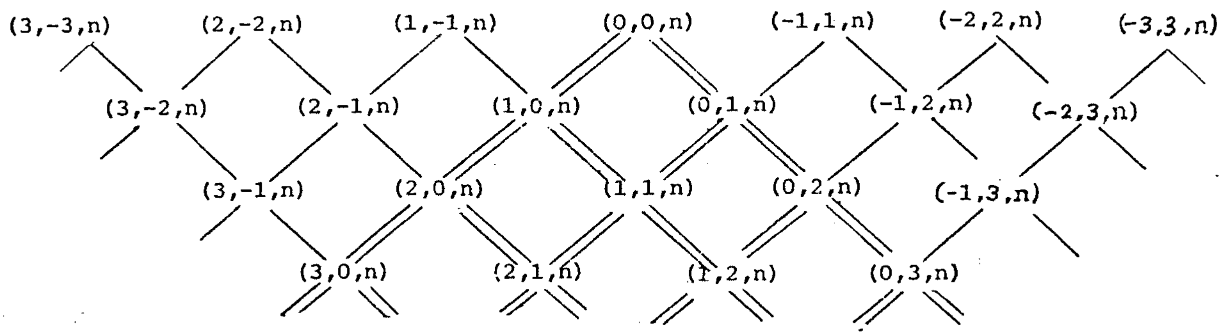


Figure 6.5.2

6.6 QUADRATIC INTERPOLATION AND EXTRAPOLATION

6.6.1 Interpolation

A general algorithm for rational interpolation has been constructed [8]. The interpolating rational function

$$R^{i}_{m,n}(x) = \frac{\sum_{j=0}^{m} a_j x^j}{\sum_{j=0}^{n} b_j x^j}$$

with $R^{i}_{m,n}(x_j) = f_j \quad j = i, i+1 \ldots i+m+n$

$$i=0,1,2\ldots$$

is expresssed and computed implicitly by

$$R^{i}_{m,n}(x) = - R^{i}_{m,n}(x) \sum_{j=1}^{n} b_j x^j + \sum_{j=0}^{m} a_j x^j$$

in which $b_0 = 1$.

This idea can be extended to quadratic approximation.

It is notationally convenient to use f(x) for the interpolating quadratic approximation.

The quadratic approximation f(x) is expressed implicitly by the equation

$$(1+a_1x + \ldots + a_\ell x^\ell) f^2(x) + (b_0+b_1x+\ldots+b_m x^m) f(x) + (\gamma_0+\gamma_1+\ldots+\gamma_n x^n) = 0 \tag{6.6.1}$$

and the interpolation is determined by requiring that (6.6.1) is satisfied at the $\ell+m+n+2$ interpolating points $x_i, x_{i+1} \ldots x_{i+\ell+m+n+1}$.

Then (6.6.1) can be expressed as

$$-f^2 = \frac{\begin{vmatrix} 0 & f_i^2 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & f_{i+\ell+m+n+1}^2 \\ xf^2 & x_i f_i^2 & \cdot & \cdot & \cdot & x_{i+\ell+m+n+1} & & & f_{i+\ell+m+n+1}^2 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ x^\ell f^2 & x_i^\ell f_i^2 & \cdot & \cdot & \cdot & x_{i+\ell+m+n+1}^\ell & & & f_{i+\ell+m+n+1}^2 \\ f & f_i & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & f_{i+\ell+m+n+1} \\ xf & x_i f_i & \cdot & \cdot & \cdot & x_{i+\ell+m+n+1} & & & f_{i+\ell+m+n+1} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ x^m f & x_i^m f_i & \cdot & \cdot & \cdot & x_{i+\ell+m+n+1}^m & & & f_{i+\ell+m+n+1} \\ 1 & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ x & x_i & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & x_{i+\ell+m+n+1} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ x^n & x_i^n & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & x_{i+\ell+m+n+1}^n \end{vmatrix}}{D} \qquad (6.6.2)$$

where D is the minor obtained by eliminating the first row and first column. $-f^2$ is expressed implicitly in terms of $\sum_{i=1}^{\ell} a_i x^i f^2(x)$, $\sum_{i=0}^{m} b_i\ x^i f(x)$ and $\sum_{i=0}^{n} \gamma_i x^i$.

This interpolation extends the two dimensional rational interpolation to three dimensions. Geometrically, given a point set $\{x_i, f(x_i)\}$ instead of constructing a curve $y = f(x)$ such that $y_i = f(x_i)$, the surfaces $z = F(x,y)$ is constructed whee $F(x,y)$ represents the right hand side of (6.6.2), and $z = y^2$, which is the left hand side of (6.6.2). These two surfaces interset in a space curve whose projection passes through (x_i, y_i). For example, given (0,5), (3,4), (4,3), (5,0) we can interpolate these points by quadratic approximations. The approximants are $(0,0,2;x)$, $(0,1,1;x)$, $(1,1,0;x)$, $(0,2,0;x)$, $(1,0,1;x)$ and $(2,0,0;x)$. The approximant $(0,0,2;x)$ gives $-f^2 = x^2 - 25$. The intersection of these two parabolic channels is a space curve whose projection on the (x,f) plane is the circle $f^2 + x^2 = 25$, which interpolates these points.

The algorithm for constructing this interpolation is an extension of the techniques in [8]. The difference between the algorithm of quadratic approximation and quadratic interpolation is that the former computes the polynomial coefficients $P(\ell,m,n;x)$ explicitly and then solves the quadratic equation, while the latter computes $-f^2$ implicitly in terms of f^2, f and x. For interpolation, we can construct $(k+1)(k+2)/2$ (where $k = \ell+m+n$) different quadratic functions whose coefficients have degrees summing to $(\ell+m+n)$ by using the $\ell+m+n+2$ interpolating points in different ways. For convenience $P^i(\ell,m,n;x)$ is now used to denote the right hand side of (6.6.2) which is determined by the interpolation points $x_i,\dots,x_{i+\ell+m+n+1}$. The functions $g_j^i(\ell,m,n;x)$ are used for computing $P^i(\ell,m,n;x)$ from $P^i(\ell-1,m,n;x)$ for $j = 1$, from $P^i(\ell,m-1,n;x)$ for $j = 2$ and from $P^i(\ell,m,n-1;x)$ for $j = 3$.

A. Basic formulas.

$$g_1^i(\ell,m,n;x) = g_1^i(\ell,m,n-1;x) - \frac{\Delta g_1^i(\ell,m,n-1;x)}{\Delta g_3^i(\ell-1,m,n;x)}\, g_3^i(\ell-1,m,n;x) \quad (6.6.3)$$

$$= g_1^i(\ell,m-1,n;x) - \frac{\Delta g_1^i(\ell,m-1,n;x)}{\Delta g_2^i(\ell-1,m,n;x)}\, g_2^i(\ell-1,m,n;x) \quad (6.6.4)$$

$$g_2^i(\ell,m,n;x) = g_2^i(\ell-1,m,n;x) - \frac{\Delta g_2^i(\ell-1,m,n;x)}{\Delta g_1^i(\ell,m-1,n;x)}\, g_1^i(\ell,m-1,n;x) \quad (6.6.5)$$

$$= g_2^i(\ell,m,n-1;x) - \frac{\Delta g_2^i(\ell,m,n-1;x)}{\Delta g_3^i(\ell,m-1,n;x)}\, g_3^i(\ell,m-1,n;x) \quad (6.6.6)$$

$$g_3^i(\ell,m.n;x) = g_3^i(\ell-1,m,n;x) - \frac{\Delta g_3^i(\ell-1,m,n;x)}{\Delta g_1^i(\ell,m,n-1,;x)}\, g_1^i(\ell,m,n-1;x) \quad (6.6.7)$$

$$g_3^i(\ell,m-1,n;x) - \frac{\Delta g_3^i(\ell,m-1,n;x)}{\Delta g_2^i(\ell,m,n-1,;x)}\, g_2^i(\ell,m,n-1;x) \quad (6.6.8)$$

where, using an abbreviated notation to denote the determinant by the elements of its k th row for $k = x,i,i+1,\ldots,i+\ell+m+n+1$,

$$g_j^{\,i}(\ell,m,n;x) = \left| x_k f_k^2 \ldots x_k^{\ell} f_k^2 \; f_k \; x_k f_k \ldots x_k^m f_k \; 1 \; x_k \ldots x_k^n \right|^T \Big/ D_j ,$$

where

$$D_1 = \left| x_k f_k^2 \;\ldots\; x_k^{\ell-1} f_k^2 \;\; f_k \;\; x_k f_k \;\ldots\; x_k^m f_k \;\; 1 \;\; x_k \;\ldots\; x_k^n \right|^T$$

$$D_2 = \left| x_k f_k^2 \;\ldots\; x_k^{\ell} f_k^2 \;\; f_k \;\; x_k f_k \;\ldots\; x_k^{m-1} f_k \;\; 1 \;\; x_k \;\ldots\; x_k^n \right|^T$$

$$D_3 = \left| x_k f_k^2 \;\ldots\; x_k^{\ell} f_k^2 \;\; f_k \;\; x_k f_k \;\ldots\; x_k^m f_k \;\; 1 \;\; x_k \;\ldots\; x_k^{n-1} \right|^T$$

$$P^i(\ell,m,n;x) = P^i(\ell-1,m,n;x) - \frac{\Delta P^i(\ell-1,m,n;x)}{\Delta g_1^i(\ell,m,n;x)} g_1^i(\ell,m,n;x) \qquad (6.6.9)$$

or

$$P^i(\ell,m,n;x) = P^i(\ell,m-1,n;x) - \frac{\Delta P^i(\ell,m-1,n;x)}{\Delta g_2^i(\ell,m,n;x)} g_2^i(\ell,m,n;x) \qquad (6.6.10)$$

or

$$P^i(\ell,m,n;x) = P^i(\ell,m,n-1;x) - \frac{\Delta P^i(\ell,m,n-1;x)}{\Delta g_3^i(\ell,m,n;x)} g_3^i(\ell,m,n;x) \qquad (6.6.11)$$

B. <u>Algorithm V.</u>

Set $N = \ell+m+n+2$.

Step 1. Initialization.

For $i = 0,1,2\ldots N-1$,

$$P^i(0,0,0;x) = -(f_i+f_{i+1})f+f_i f_{i+1}$$

$$g_j^i(0,0,0;x) = f-f_i \quad \text{for } j = 1,2,3.$$

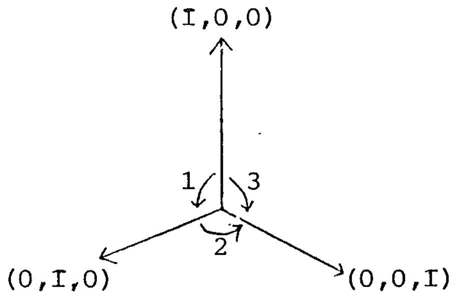


Figure 6.6.1.

For $k = 1,2\ldots N-2$;

For dimension 1 in figure 6.6.1

$$g_1^i(-k,k,0;x) = g_2^i(-k,k,0;x) = x^k f - x_i^k f_i,$$

$$g_1^i(k,-k,0;x) = g_2^i(k,-k,0;x) = x^k f^2 - x_i^k f_i^2,$$

For dimension 2.

$$g_2^i(0,-k,k;x) = g_3^i(0,-k,k;x) = x^k - x_i^k$$

$$g_2^i(0,k,-k;x) = g_3^i(0,k,-k;x) = x^k f - x_i^k f_i$$

For dimension 3.

$$g_1^i(-k,0,k;x) = g_3^i(-k,0,k;x) = x^k - x_i^k$$

$$g_1^i(k,0,-k;x) = g_3^i(k,0,-k;x) = x^k f^2 - x_i^k f_i^2$$

Remark: In order to express the dimension and array clearly the initialization is repeated for $(0,0,I)$, $(0,I,0)$ and $(I,0,0)$. When the computation is done, one just need to compute once and redefine in different array for convenience.

Step 2. Dimension 1.

For $\ell,m=0, \pm 1, \pm 2, \pm N-2$ and $\ell + m \neq 0$

compute $g_1^i(\ell,m,0;x)$ by (6.6.4)

and $g_2^i(\ell,m,0;x)$ by (6.6.5).

For $\ell,m \geqslant 0$

compute $p^i(\ell,m,0;x)$ by (6.6.9) or (6.6.10).

Dimension 2.

For $m,n = 0, \pm 1, \pm 2, \pm N-2$ and $m+n \neq 0$

compute g_2^i $(0,m,n;x)$ by (6.6.6) and

g_3^i $(0,m,n;x)$ by (6.6.8).

For $m,n \geqslant 0$

compute $P^i(0,m,n;x)$ by (6.6.10) or (6.6.11).

Dimension 3.

For $\ell,n = 0, \pm 1, \pm 2, \pm N-2$ and $\ell + n \neq 0$

compute $g_1^i(\ell,0,n;x)$ by (6.6.3) and $g_3^i(\ell,0,n;x)$ by (6.6.7).

For $\ell,m \geqslant 0$.

compute $P^i(\ell,0,n;x)$ by (6.6.9) and (6.6.11).

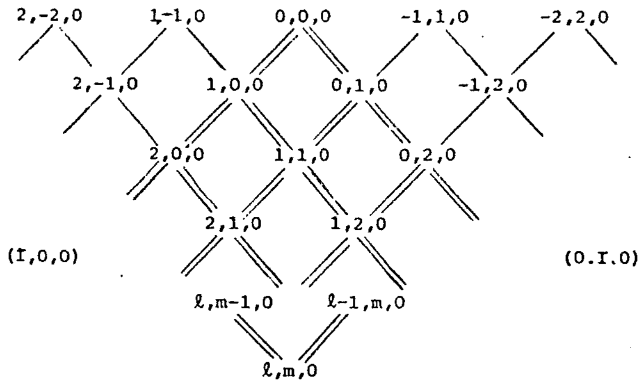
For $\ell,m,n \geqslant 0,1,2...$

and $j = 1,2,3$

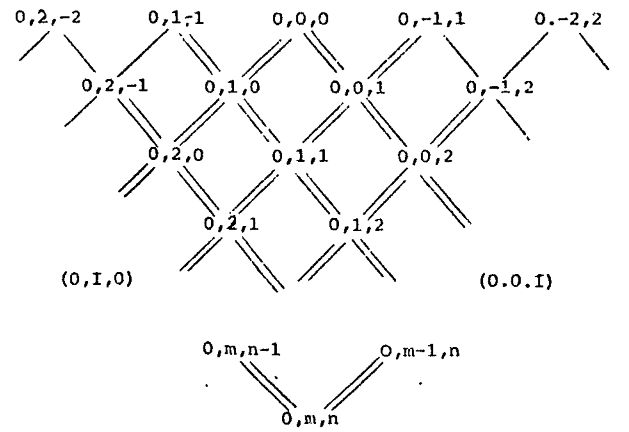
compute $g_j^i(\ell,m,n;x)$ from (6.6.3 - 6.6.8).

and compute $P^i(\ell,m,n;x)$ from one of (6.6.9 - 6.6.11).

By using the above algorithm, the arrays of the three dimensions can be constructed as shown in figures 6.6.2a – d .



(a)



(b)

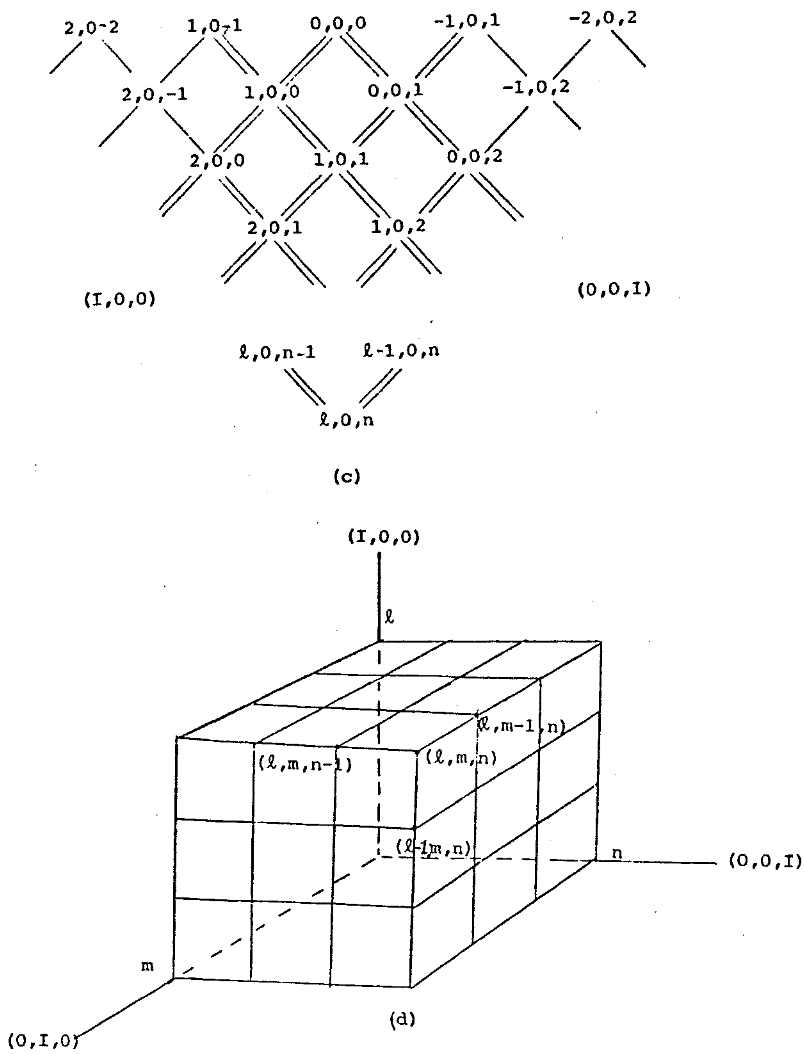


Figure 6.6.2

Notes: 1. $g_j^i(\ell,m,n;x)$ where $j = 1,2,3$ have the same numerators and the denominators have one row different.

2. $g_2^i(\ell-1,m,n;x)$ and $g_1^i(\ell,m-1,n;x)$; $g_2^i(\ell,m,n-1;x)$ and $g_3^i(\ell,m-1,n;x)$; $g_1^i(\ell,m,n-1;x)$ and $g_3^i(\ell-1,m,n;x)$ have the same denominators but the numerators have one row different.

3. In theory, the derivative of $g_j^i(\ell,m,n;x)$, for example $g_1^i(\ell,m,n;x)$ is

$$g_1^i(\ell,m,n;x) = \frac{\Delta g_1^i(\ell,m,n-1;x)}{\Delta g_3^i(\ell-1,m,n;x)} \; g_3^i(\ell-1,m,n;x) - g_1^i(\ell,m,n-1;x) \; .$$

The difference between the above expression and (6.6.3) is only the negative sign. In the algorithm, the derivatives of $g_j^i(\ell,m,n;x)$ are unified so that (6.6.8) have the same form as $P^i(\ell,m,n;x)$ (6.6.9 - 6.6.11).

6.6.2 Extrapolation

This process also leads to a generalization of polynomial (Richardson) and rational extrapolation applies to a sequence $\{S_n\}$ whose terms satisfy $S_n = S(^1/n)$. $S(x)$ is approximated by an interpolating quadratic approximation and the extrapolated value, $S(0)$, is found by evaluating (6.6.1) at $x = 0$. In this case only b_0 and γ_0 in (6.6.1) are needed to be computed by the above algorithm.

For simplification we write $b_0^i(\ell,m,n;0) = b_0^i(\ell,m,n)$, $\gamma_0^i(\ell,m,n;0) = \gamma_0^i(\ell,m,n)$ and $g_j^i(\ell,m,n;0) = g_j^i(\ell,m,n)$. $\gamma_0^i(\ell,m,n)$ and $b_0^i(\ell,m.n)$ can be obtained explicitly from (6.6.1).

$$\gamma_0^i(\ell,m,n) = \frac{\begin{vmatrix} x_i f_i^2 \cdots x_i^{\ell} f_i^2 & f_i & x_i f_i \cdots x_i^m f_i & -f_i^2 x_i & \cdots & x_i^n \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ x_k f_k^2 \cdots x_k^{\ell} f_k^2 & f_k & x_k f_k \cdots x_k^m f_k & -f_k^2 x_k & \cdots & x_k^n \end{vmatrix}}{\begin{vmatrix} x_i f_i^2 \cdots x_i^{\ell} f_i^2 & f_i & x_i f_i \cdots x_i^m f_i & 1 & x_i & \cdots & x_i^n \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ x_k f_k^2 \cdots x_k^{\ell} f_k^2 & f_k & x_k f_k \cdots x_k^m f_k & 1 & x_k & \cdots & x_k^k \end{vmatrix}}$$

where $k = i + \ell+m+n+1$.

If each row (except the first row) is replaced by its difference with the preceding one, and the $(\ell+m+2)$th column is shifted to the first column, then

$$\gamma_0^i(\ell,m,n) = -\frac{\begin{vmatrix} f_i^2 & x_i f_i^2 & \cdots & x_i^\ell f_i^2 & f_i & x_i f_i & \cdots & x_i^m f_i & x_i & \cdots & x_i^n \\ \Delta f_i & \Delta x_i f_i^2 & \cdots & \Delta x_i^\ell f_i^2 & \Delta f_i & \Delta x_i f_i & \cdots & \Delta x_i^m f_i & \Delta x_i & \cdots & \Delta x_i^n \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \Delta f_k^2 & \Delta x_k f_k^2 & \cdots & \Delta x_k^\ell f_k^2 & \Delta f_k & \Delta x_k f_k & \cdots & \Delta x_k^m f_k & \Delta x_k & \cdots & \Delta x_k^n \end{vmatrix}}{D.}$$

where $k = i+\ell+m+n$ and D is the minor obtained by eliminating the first row and the first column. Also

$$b_0^i(\ell,m,n) = \frac{\begin{vmatrix} x_i f_i^2 & \cdots & x_i^\ell f_i^2 & -f_i^2 & x_i f_i & \cdots & x_i^m f_i & x_i & \cdots & x_i^n \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ x_k f_k^2 & \cdots & x_k^\ell f_k^2 & -f_k^2 & x_k f_k & \cdots & x_k^m f_k & x_k & \cdots & x_k^n \end{vmatrix}}{\begin{vmatrix} x_i f_i^2 & \cdots & x_i^\ell f_i^2 & f_i & x_i f_i & \cdots & x_i^m f_i & x_i & \cdots & x_i^n \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ x_k f_k^2 & \cdots & x_k^\ell f_k^2 & f_k & x_k f_k & \cdots & x_k^m f_k & x_k & \cdots & x_k^n \end{vmatrix}}$$

where $k = i+\ell+m+n+1$.

Again from second row on, each row is replaced by its difference with the preceding one, the $(\ell+1)$th columns is shifted to the first column, and $(1,\Delta f_i \ldots \Delta f_k)^T$ is added to the $(\ell+2)$th column, then

$$b_0^i(\ell,m,n) = \frac{(-1)(-1)^{\ell}(-1)^{\ell+1} \begin{vmatrix} 0 & \cdots & 0 & 1 & 0 & \cdots & \cdots & \cdots & 0 \\ \Delta f_i^2 & \Delta x_i f_i^2 \cdots & \Delta x_i^{\ell} f_i^2 & \Delta f_i & \Delta x_i f_i \cdots & \Delta x_i^m f_i & \Delta x_i \cdots & \Delta x_i^n \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \Delta f_k^2 & \Delta x_k f_k^2 \cdots & \Delta x_k^{\ell} f_k^2 & \Delta f_k & \Delta x_k f_k \cdots & \Delta x_k^m f_k & \Delta x_k \cdots & \Delta x_k^n \end{vmatrix}}{D}$$

where $k = i+\ell+m+n$.

The algorithm for computing $b_0^i(\ell,m,n)$ and $\gamma_0^i(\ell,m,n)$ is the same as algorithm V. $P^i(\ell,m,n)$ is used to compute the coefficients $b_0^i(\ell,m,n)$ and $\gamma_0^i(\ell,m,n)$. ${}_{b_0}g_j^i(\ell,m,n)$ and ${}_{\gamma_0}g_j^i(\ell,m,n)$ are used to compute $b_0^i(\ell,m,n)$ and $\gamma_0^i(\ell,m,n)$ from $b_0^i(\ell-1,m,n)$ and $\gamma_0^i(\ell-1,m,n)$ for $j = 1$, from $b_0^i(\ell,m-1,n)$ and $\gamma_0^i(\ell,m-1,n)$ for $j = 2$ and from $b_0^i(\ell,m,n-1)$ and $\gamma_0^i(\ell,m,n-1)$ for $j = 3$ respectively.

Algorithm VI

Set $N = \ell+m+n+2$.

Step 1. Initialization

For $i = 0,1,2...N-2$

$$b_0^i(0,0,0) = \frac{\begin{vmatrix} 0 & 1 \\ \Delta f_0^2 & \Delta f_0 \end{vmatrix}}{\Delta f_0}$$

$$\gamma_0^i(0,0,0) = -\frac{\begin{vmatrix} \Delta f_0^2 & f_0 \\ \Delta f_0^2 & \Delta f_0 \end{vmatrix}}{\Delta f_0}$$

$${}^{b_0}_{\gamma_0}g_j^i(0,0,0) = \frac{1}{f_i} \quad \text{for } j = 1,2,3.$$

For k = 1,2,3...N-2

For dimension 1 on figure (6.6.2)

$$\begin{matrix} b_0 \\ \gamma_0 \end{matrix} g_1^{i}(-k,k,0) = \begin{matrix} b_0 \\ \gamma_0 \end{matrix} g_2^{i}(-k,k,0) = \begin{matrix} x_i^{k} f_i \\ 0 \end{matrix}$$

$$\begin{matrix} b_0 \\ \gamma_0 \end{matrix} g_1^{i}(k,-k,0) = \begin{matrix} b_0 \\ \gamma_0 \end{matrix} g_2^{i}(k,-k,0) = \begin{matrix} x_i^{k} f_i^{2} \\ 0 \end{matrix}$$

For dimension 2

$$\begin{matrix} b_0 \\ \gamma_0 \end{matrix} g_2^{i}(0,-k,k) = \begin{matrix} b_0 \\ \gamma_0 \end{matrix} g_3^{i}(0,-k,k) = \begin{matrix} x_i^{k} \\ 0 \end{matrix}$$

$$\begin{matrix} b_0 \\ \gamma_0 \end{matrix} g_2^{i}(0,k,-k) = \begin{matrix} b_0 \\ \gamma_0 \end{matrix} g_3^{i}(0,k,-k) = \begin{matrix} x_i^{k} f_i \\ 0 \end{matrix}$$

For dimension 3

$$\begin{matrix} b_0 \\ \gamma_0 \end{matrix} g_1^{i}(-k,0,k) = \begin{matrix} b_0 \\ \gamma_0 \end{matrix} g_3^{i}(-k,0,k) = \begin{matrix} x_i^{k} \\ 0 \end{matrix}$$

$$\begin{matrix} b_0 \\ \gamma_0 \end{matrix} g_1^{i}(k,0,-k) = \begin{matrix} b_0 \\ \gamma_0 \end{matrix} g_3^{i}(k,0,-k) = \begin{matrix} x_i^{k} f_i^{2} \\ 0 \end{matrix}$$

Step 2. Same as step 2 of algorithm V but each one has to be used twice for computing b_0 and γ_0.

6.7 NUMERICAL EXAMPLES

Example 1 : Quadratic approximation of e^{x}.

Table 6.7.1

(x_1 and x_2 refer to the 2 roots of the quadratic)

ℓ	m	n	α	β	γ	Value at x = 1	Exact value (2.7182818)
						x_1	x_2
0	0	0	1	-2	1	1	
		1	1	-4	$3+2x$	-	
		2	1	-8	$7+6x+2x^2$	3	
		3	1	-16	$15+14x+6x^2+\frac{4}{3}x^3$	2.7400887	
		4	1	-32	$31+30x+14x^2+4x^3+\frac{2}{3}x^4$	2.7209438	
1	0	0	$1-\frac{2}{3}x$	$-\frac{4}{3}$	$\frac{1}{3}$		3.7320508
		1	$1-\frac{1}{2}x$	-2	$1+\frac{1}{2}x$		3
		2	$1-\frac{2}{5}x$	$-\frac{16}{5}$	$\frac{11}{5}+\frac{8}{5}x+\frac{2}{5}x^2$		3
		3	$1-\frac{1}{3}x$	$-\frac{16}{3}$	$\frac{13}{3}+\frac{11}{3}x+\frac{4}{3}x^2+\frac{2}{9}x^3$	2.7090056	
0	1	0	1	$-2x$	-1		2.4142136
		1	1	$4-4x$	$-5-2x$		2.6457513
		2	1	$16-8x$	$-17-10x-2x^2$		2.7082039
		3	1	$48-16x$	$-49-34x-10x^2-\frac{4}{3}x^3$		2.7171935

Table 6.7.1 (continued)

ℓ	m	n	α	β	γ	x_1	x_2
2	0	0	$1-\frac{6}{7}x+\frac{2}{7}x^2$	$-\frac{8}{7}$	$\frac{1}{7}$		2.5351838
		1	$1-\frac{8}{11}x+\frac{2}{11}x^2$	$-\frac{16}{11}$	$\frac{5}{11}+\frac{2}{11}x$		2.6770320
		2	$1-\frac{5}{8}x+\frac{1}{8}x^2$	-2	$1+\frac{5}{8}x+\frac{1}{8}x^2$		2.7071068
1	1	0	$1-\frac{2}{5}x$	$-\frac{4}{5}-\frac{4}{5}x$	$-\frac{1}{5}$		2.7862996
		1	$1-\frac{1}{3}x$	$-\frac{4}{3}x$	$-1-\frac{1}{3}x$		2.7320507
		2	$1-\frac{2}{7}x$	$-\frac{16}{7}+\frac{16}{7}x$	$-\frac{23}{7}-\frac{12}{7}x-\frac{2}{7}x^2$		2.7202941
0	2	0	1	$-2-x^2$	1		2.6180340
		1	1	$-8+4x-2x^2$	$7+2x$	3	3
		2	1	$-32+16x-4x^2$	$31+14x+2x^2$	2.7198901	

Table 6.7.1 (continued)

ℓ	m	n	α	β	γ	x_1	x_2
3	0	0	$1-\frac{14}{15}x+\frac{2}{5}x^2-\frac{4}{45}x^3$	$-\frac{16}{15}$	$\frac{1}{15}$		2.7843137
		1	$1-\frac{11}{13}x+\frac{4}{13}x^2-\frac{6}{117}x^3$	$-\frac{16}{13}$	$\frac{3}{13}+\frac{1}{13}x$		2.7843137
2	1	0	$1-\frac{10}{17}x+\frac{2}{17}x^2$	$-\frac{16}{17}-\frac{8}{17}x$	$-\frac{1}{17}$		2.7077418
		1	$1-\frac{12}{23}x+\frac{2}{23}x^2$	$-\frac{16}{23}-\frac{16}{23}x$	$-\frac{7}{23}-\frac{2}{23}x$		2.7164006
1	2	0	$1-\frac{2}{7}x$	$-\frac{8}{7}-\frac{4}{7}x-\frac{2}{7}x^2$	$\frac{1}{7}$		2.7266500
		1	$1-\frac{1}{4}x$	$-2-\frac{1}{2}x^2$	$1+\frac{1}{4}x$		2.7032574
0	3	0	1	$-2x-\frac{1}{3}x^3$	-1		2.7032574
		1	1	$8-8x+2x^2-\frac{2}{3}x^3$	$-9-2x$		2.7162972
4	0	0	$1-\frac{30}{31}x+\frac{14}{31}x^2-\frac{4}{31}x^3+\frac{2}{93}x^4$	$\frac{32}{31}$	$\frac{1}{31}$	2.7112428	
3	1	0	$1-\frac{409}{833}x+\frac{349}{1666}x^2-\frac{17}{588}x^3$	$-\frac{818}{833}-\frac{529}{1666}x$	$-\frac{15}{833}$		2.7206005
2	2	0	$1-\frac{14}{31}x+\frac{2}{31}x^2$	$-\frac{32}{31}-\frac{16}{31}x-\frac{4}{31}x^2$	$\frac{1}{31}$		2.7174743
1	3	0	$1-\frac{2}{9}x$	$-\frac{8}{9}-\frac{8}{9}x-\frac{2}{9}x^2-\frac{2}{27}x^3$	$-\frac{1}{9}$		2.7192031
0	4	0	1	$-2-x^2-\frac{1}{12}x^4$	1		2.7150107
.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.

Let k be the total (or highest) degree of the quadratic approximant $(\ell,m,n;x)$. From the above results, for each k, (ℓ,m,n) in table 6.7.2 gives the best approximation of e^1 .

Table 6.7.2

k	$(\ell,m,n;x)$	e^1
1	0 1 0	2.4142136
2	1 1 0	2.7862996
3	1 2 0	2.7266500
4	2 2 0	2.7174743
5	2 3 0	2.7182188
6	3 3 0	2.7182863

Example 2 : Quadratic approximation is used to accelerate the convergence of sequences of numerical approximants to various integrals with singularities (of the integrands or their derivatives) at the end point. The values were obtained using algorithm III (or IV) described in section 6.5.

The sequences of approximants are the trapezoidal rule approximations of the integrals. The singularities of the integrand, f(x), are ignored. The tables 6.7.3 - 6.7.4 give the absolute error of the best quadratic extrapolation value, where the root is either (1) $x_1 = (-\beta-\sqrt{\beta^2-4\alpha\gamma})/2\alpha$ or (2) $x_2 = -2\gamma/(\beta+\sqrt{\beta^2-4\alpha\gamma})$ and the error of the value from the ε-algorithm. The comparison is between approximations using the same number of terms of the sequence. (The computations are accurate to nine decimal places).

The integrands in table 6.7.3 have singularities in their first derivatives and the integrands in table 6.7.4 have singularities at one (or both) of the endpoints.

As can be seen from tables 6.7.3 and 6.7.4, by using the same number of terms for both algorithms, the ε-algorithm gives slightly better results for the lower degree ($\leqslant 6$) approximation, but for higher degrees, quadratic approximation is as good as the ε-algorithm. The functions $f(x) = x \ell n\, x$, $x^{\frac{1}{2}} \ell n\, x$ and $\ell n\, x(\ell n|x-0.3|)(1-x)^{-0.56}$ are in general favourable to the quadratic approximation. The reason is not immediately known but it is conjectured that the quadratic algorithm is good for the higher degree approximation and for integrands with more singularities.

Table 6.7.3

$|\text{Error}| = |\mathcal{I} f - \text{Approx. of quadratic}/\varepsilon\text{-algorithm}|$ for $\mathcal{I} f = \int_0^1 f(x)dx$

	$f(x) = x^{\frac{1}{2}}$	$f(x) = x \ln x$	$f(x) = x^{\frac{1}{2}} \ln x$	$f(x) = x \ln^3 x$	$f(x) = x \ln^8 x$
	/ (1,1) = 0.32×10^{-3}	(0,1,0) = 0.18×10^{-3} (1) (1,1) = 0.34×10^{-3}	(0,1,0) = 0.18×10^{-2} (1) (1,1) = 0.32×10^{-2}	(0,1,0) = 0.11×10^{0} (1) (1,1) = 0.10×10^{0}	(0,4,1) = 0.42×10^{2} (1) (3,3) = 0.43×10^{3}
	(1,1,0) = 0.29×10^{-4} (1) (1,2) = 0.77×10^{-4}	(0,1,1) = 0.39×10^{-4} (1) (1,2) = 0.71×10^{-4}	(2,0,0) = 0.74×10^{-4} (1) (1,2) = 0.10×10^{-2}	(0,1,1) = 0.30×10^{-1} (1) (1,2) = 0.14×10^{-1}	(0,3,3) = 0.31×10^{2} (1) (3,4) = 0.11×10^{2}
	(1,1,1) = 0.95×10^{-6} (1) (2,2) = 0.39×10^{-6}	(3,0,0) = 0.26×10^{-6} (1) (2,2) = 0.32×10^{-6}	(2,0,1) = 0.65×10^{-5} (1) (2,2) = 0.26×10^{-4}	(0,1,2) = 0.62×10^{-2} (1) (2,2) = 0.87×10^{-3}	(3,4,0) = 0.10×10^{2} (1) (4,4) = 0.20×10^{1}
	(2,0,2) = 0.14×10^{-6} (1) (2,3) = 0.25×10^{-7}	(2,1,1 = 0.53×10^{-7} (1) (2,3) = 0.20×10^{-8}	(4,0,0) = 0.36×10^{-6} (1) (2,3) = 0.53×10^{-5}	(0,2,2) = 0.43×10^{-3} (2) (2,3) = 0.18×10^{-3}	(0,3,5) = 0.19×10^{1} (1) (4,5) = 0.21×10^{0}
	(2,0,3) = 0.68×10^{-8} (1) (3,3) = 0.10×10^{-9}	(0,3,2) = 0.10×10^{-9} (1) (3,3) = 0.24×10^{-8}	(3,1,1) = 0.11×10^{-7} (1) (3,3) = 0.47×10^{-8}	(0,2,3 = 0.54×10^{-4} (2) (3,3) - 0.24×10^{-5}	(0.5.4) = 0.37×10^{0} (1) (5,5) = 0.22×10^{-1} (1)
	(3,0,3) = 0.90×10^{-9} (1) (3,4) = 0.11×10^{-8}	(0.4.2) = 0.56×10^{-8} (1) (3,4) = 0.21×10^{-8}	(2,2,2) = 0.43×10^{-8} (1) (3,4) = 0.50×10^{-8}	(0,3,3) = 0.84×10^{-6} (1) (3,4) = 0.33×10^{-6}	(0,5,5) = 0.23×10^{-1} (5,6) = 0.23×10^{-2}
	(4,1,2) = 0.14×10^{-8} (1) (4,4) = 0.15×10^{-8}	(0,4,3) = 0.10×10^{-9} (1) (4,4) = 0.40×10^{-9}	(2,3,2) = 0.10×10^{-8} (1) (4,4) = 0.48×10^{-8}	(0,4,3) = 0.10×10^{-9} (1) (4,4) = 0.21×10^{-8}	(0,7,4) = 0.81×10^{-3} (1) (6,6) = 0.13×10^{-3}
	(4,0,4) = 0.11×10^{-8} (1) (4,5) = 0.11×10^{-8}	(0,4,4) = 0.10×10^{-9} (2) (4,5) = 0.50×10^{-9}	(5.1.2) = 0.12×10^{-8} (1) (4,5) = 0.16×10^{-8}	(0,4,4) = 0.10×10^{-9} (1) (4,5) = 0.17×10^{-8}	(0,8,4) = 0.10×10^{-4} (1) (6,7) = 0.15×10^{-4}
	(5,0,4) = 0.21×10^{-8} (1) (5,5) = 0.50×10^{-9}	(0,5,4) = 0.10×10^{-9} (1) (5,5) = 0.10×10^{-9}	(4,3,2) = 0.28×10^{-9} (2) (5,5) = 0.14×10^{-8}	(0,5,4) - 0.10×10^{-9} (2) (5,5) = 0.18×10^{-8}	(0,6,7) = 0.86×10^{-5} (2) (7,7) = 0.11×10^{-4}
	(5,0,5) = 0.16×10^{-9} (1) (5,6) = 0.10×10^{-9}	(0,6,4) = 0.10×10^{-9} (1) (6,5) = 0.10×10^{-9}	(2,5,3) = 0.26×10^{-8} (2) (5,5) = 0.21×10^{-8}	(0,5,5) - 0.10×10^{-9} (1) (5,6) = 0.17×10^{-8}	(0,9,5) = 0.11×10^{-4} (1) (7,8) = 0.16×10^{-4}
EXACT	2/3	- 1/4	- 4/9	- 3/8	-315/4

Note: The dash means there is no real root for that term in the table. For $f(x) = x \ln^8 x$, the sequence of approximations converges slowly. The comparison of the extrapolation starts from using seven terms.

Table 6.7.4

|Error = $I f$ - Approx. of quadratic / ε-algorithm| for $I f = \int_0^1 f(x)dx$

	$f(x) = x^{-\frac{1}{2}}$	$f(x) = x^{-\frac{1}{2}} \ell n\, x$	$f(x) = (x^2 - 0.0.1)^{-1}$	$f(x) = \ell n x\, (\ell n\lvert x-0.3\rvert)(1-x)^{-0.56}$
	(1,1) = 0.23×10^{-1}	(0,1,0) = 0.17×10^{1} (1) (1,1) = 0.16×10^{2}	(1,1) = 0.42×10^{-3}	(0,1,0) = 0.62×10^{0} (1) (1,1) = 0.51×10^{1}
	(1,0,1) = 0.11×10^{-1} (1) (1,2) = 0.62×10^{-2}	(0,1,1) = 0.13×10^{1} (1) (1,2) = 0.25×10^{1}	(0,1,1) = 0.21×10^{-3} (1) (1,2) = 0.11×10^{-3}	(0,1,1) = 0.24×10^{-3} (1) (2,1) = 0.93×10^{-2}
	(1,1,1) = 0.27×10^{-3} (1) (2,2) = 0.44×10^{-4}	(1,1,1) = 0.44×10^{0} (1) (2,2) = 0.15×10^{0}	(1,1,1) = 0.25×10^{-6} (2) (2,2) = 0.19×10^{-6}	(0,1,2) = 0.32×10^{-3} (1) (2,2) = 0.51×10^{-2}
	(2,2,0) = 0.27×10^{-4} (1) (2,3) = 0.30×10^{-5}	(2,1,1) = 0.42×10^{-1} (1) (2,3) = 0.34×10^{-1}	(2,1,1) = 0.39×10^{-7} (2) (2,3) = 0.23×10^{-7}	(1,1,2) - 0.20×10^{-3} (1) (2,3) = 0.13×10^{-2}
	(3,2,0) = 0.18×10^{-5} (1) (3,3) = 0.45×10^{-7}	(2,1,2) = 0.42×10^{-2} (1) (3,3) = 0.69×10^{-3}	(1,2,1) = 0.39×10^{-7} (1) (3,3) = 0.41×10^{-7}	(1,1,3) = 0.42×10^{-4} (1) (3,3) = 0.23×10^{-3}
	(2,4,0) = 0.47×10^{-7} (1) (3,4) = 0.67×10^{-7}	(4,2,0) = 0.76×10^{-4} (1) (3,4) = 0.45×10^{-4}	(0,3,3) = 0.65×10^{-8} (2) (3,4) = 0.40×10^{-7}	(3,3,0) = 0.11×10^{-5} (1) (3,4) = 0.26×10^{-5}
	(2,3,2) = 0.51×10^{-7} (1) (4,4) = 0.36×10^{-8}	(0,4,3) = 0.50×10^{-4} (2) (4,4) = 0.13×10^{-5}	(3,1,3) = 0.53×10^{-7} (2) (4,4) = 0.50×10^{-7}	(0,4,3) = 0.85×10^{-8} (2) (4,4) = 0.59×10^{-7}
	(0,4,4) = 0.19×10^{-8} (2) (4,5) = 0.31×10^{-8}	(4,3,1) = 0.13×10^{-6} (1) (4,5) = 0.12×10^{-5}	(2,3,3) = 0.51×10^{-8} (2) (4.5) = 0.24×10^{-8}	(0,4,4) = 0.18×10^{-6} (1) (4,5) = 0.27×10^{-7}
	(5.0.4) = 0.20×10^{-8} (1) (5,5) = 0.37×10^{-8}	(3,2,4) - 0.28×10^{-5} (1) (5,5) = 0.10×10^{-8}	(4,0,5) = 0.12×10^{-8} (2) (5,5) = 0.10×10^{-8}	(3,6,0) = 0.59×10^{-7} (1) (5,5) = 0.49×10^{-7}
	(2,5,3) = 0.95×10^{-9} (1) (5,6) = 0.20×10^{-8}	(0,6,4) = 0.47×10^{-6} (1) (5,6) = 0.13×10^{-6}	(1,6,3) = 0.16×10^{-8} (5,6) = 0.29×10^{-8}	(0,2,8) = 0.29×10^{-7} (2) (5,6) = 0.63×10^{-7}
EXACT	2	-4	-1.0033535	2.35878125

Example 3. Quadratic interpolation. The results are calculated in implicit form using algorithm V from section 6.6.

Table 6.7.5.

i	x_i	f_i	(0,0,1)	(0,1,0)	(1,0,0)
0	0	1			
1	1	0			
2	2	1	$f^2-f=0$	$f^2-f=0$	$f^2-f=0$
3	3	2	-	$f^2+f(1-x) = 0$	$f^2(1-\frac{1}{4}x)-\frac{1}{2}f=0$
4	4	4	$f^2-9f+6x-4=0$	$f^2+f(9-3x)-4=0$	$f^2(1-\frac{3}{16}x)-\frac{9}{8}f+\frac{4}{8}=0$

(0,0,2)	(0,2,0)	(2,0,0)
$f^2-(1-x^2) = 0$	$f^2-(1-\frac{2}{3}x+\frac{1}{3}x^2)f = 0$	$f^2(1+\frac{1}{3}x-\frac{1}{6}x^2)-f=0$
$f^2-7f+(-8+9x-x^2) = 0$	$f^2-(2-\frac{3}{2}x+\frac{1}{2}x^2)f = 0$	$f^2(1-\frac{9}{22}x+\frac{1}{22}x^2)-\frac{4}{11}f=0$

(0,1,1)	(1,0,1)	(1,1,0)
$f^2-xf-(1-x)=0$	$f^2(1-\frac{1}{4}x)-\frac{3}{4}f-(\frac{1}{4}-\frac{1}{4}x)=0$	$f^2(1-\frac{1}{6}x) - (1-\frac{1}{6}x)f=0$
$f^2-(3+x)f-(4-4x)=0$	$f^2(1-\frac{1}{4}x)+\frac{3}{2}f+(2-2x)=0$	$f^2(1-\frac{1}{6}x)-\frac{1}{3}xf=0$

(1,1,1)
$f^2(7-x)-(3+3x)f-(4-4x)=0$

Example 4. Comparison of acceleration of slowly convergent sequence by quadratic approximation (section 6.5) and by quadratic interpolation (section 6.6).

Consider a sequence $\{f_i\}$ of approximations to $-\int_0^1 x\ \ell n^3\ x\ dx = 0.375$ using trapexoidal rule on 2^i intervals for $i = 1(1)14$.

Table 6.7.6

i	x_i	f_i
1	0.5	0.083256263
2	0.25	0.212604567
3	0.125	0.299399300
4	0.625×10^{-1}	0.343536435
5	0.3125×10^{-1}	0.362877208
6	0.15625×10^{-1}	0.370585398
7	0.78125×10^{-2}	0.373460290
8	0.390625×10^{-2}	0.374480996
9	0.1953125×10^{-2}	0.374829829
10	0.9765625×10^{-3}	0.374945468
11	$0.48828125 \times 10^{-3}$	0.374982859
12	$0.244140625 \times 10^{-3}$	0.374994700
13	$0.1220703125 \times 10^{-3}$	0.374998385
14	$0.6103515625 \times 10^{-4}$	0.374999514

The tables (6.7.7-6.7.10) give the numbers of significant digits of (i) quadratic interpolation and (ii) quadratic approximation for the same number of terms of sequence $\{f_i\}$.

Both methods increase the number of significant digits of the original sequence. Quadratic approximation is superior to quadratic interpolation and also involves less computation.

Table 6.7.7

	(i)				(ii)	
i	(1,0,0)	(0,1,0)	(0,0,1)	n	(0,1,n)	(1,0,n)
1	0	1	0	0	0	0
2	1	1	1	1	1	0
3	1	1	1	2	1	0
4	2	2	2	3	2	1
5	2	2	2	4	3	2
6	3	3	3	5	4	4
7	3	3	3	6	4	4
8	4	4	4	7	5	4
9	4	4	4	8	6	5
10	5	5	5	9	6	5
11	5	5	5	10	7	6
12	6	6	6	11	8	7
13	7	7	7	12	8	7

Table 6.7.8

	(i)							(ii)		
i	(2,0,0)	(1,1,0)	(0,2,0)	(1,0,1)	(0,1,1)	(0,0,2)	n	(0.2.n)	(1,1,n)	(2,0,n)
1	1	1	1	2	1	0	0	1	0	0
2	2	2	2	2	1	1	1	2	1	1
3	2	2	2	3	2	1	2	3	2	2
4	3	3	3	3	3	3	3	4	3	3
5	3	3	3	4	3	3	4	5	4	3
6	4	4	4	4	4	3	5	5	5	3
7	4	4	4	5	4	4	6	6	5	3
8	5	5	5	5	5	4	7	7	6	5
9	5	5	5	6	5	5	8	8	7	6
10	6	6	6	6	6	5	9	8	7	6
11	6	6	6	6	6	6	10	9	8	7
12	7	6	7	6	7	6	11	9	9	8

Table 6.7.9

	(i)											(ii)			
i	(3,0,0)	(2,1,0)	(1,2,0)	(0,3,0)	(2,0,1)	(1,1,1)	(0,2,1)	(1,0,2)	(0,1,2)	(0,0,3)	n	(0,3,n)	(1,2,n)	(2,1,n)	(3,0,n)
1	2	2	1	2	2	2	2	2	1	2	0	1	2	2	0
2	2	3	3	3	2	2	2	2	2	2	1	3	2	3	2
3	2	3	3	3	3	3	2	3	3	3	2	5	3	4	3
4	3	4	4	3	4	3	4	4	4	4	3	6	4	4	4
5	4	4	4	4	4	4	4	4	4	4	4	6	5	5	5
6	4	5	5	4	5	4	5	5	5	4	5	8	6	6	6
7	6	5	5	6	5	5	5	5	5	5	6	7	7	6	6
8	6	6	6	6	6	5	6	6	6	6	7	8	8	7	7
9	6	6	6	6	6	-	6	6	6	6	8	8	8	9	8
10	7	7	7	7	7	-	7	7	7	7	9	8	8	8	8
11	7	7	7	8	7	-	7	7	7	6	10	9	9	8	8

Table 6.7.10

	(i)																(ii)				
i	(4,0,0)	(3,1,0)	(2,2,0)	(1,3,0)	(0,4,0)	(3,0,1)	(2,1,1)	(1,2,1)	(0,3,1)	(2,0,2)	(1,1,2)	(0,2,2)	(1,0,3)	(0,1,3)	(0,0,4)	n	(0,4,n)	(1,3,n)	(2,2,n)	(3,1,n)	(4,0,n)
1	2	2	3	3	2	3	-	3	2	-	-	-	3	3	3	0	2	2	3	3	1
2	3	3	3	3	3	5	4	3	3	4	3	3	3	3	3	1	5	3	4	5	4
3	3	4	4	4	3	4	4	4	4	4	4	4	4	4	3	2	6	5	4	6	5
4	4	4	4	4	4	5	4	4	4	4	4	4	4	4	4	3	9	6	3	6	6
5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	4	9	7	6	7	7
6	5	5	5	5	5	6	5	5	5	5	5	5	5	5	5	5	6	8	7	7	8
7	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	8	8	9	8	9
8	6	6	6	6	6	6	6	6	6	6	7	6	6	6	6	7	9	7	7	8	9
9	7	8	5	7	7	7	5	5	7	6	5	5	7	7	7	8	9	9	8	8	7
10	6	6	-	7	6	6	-	-	6	6	-	5	6	7	6	9	8	8	8	8	8

6.8 CONCLUSION

This chapter considers the extension of the Pade approximation to a higher dimension motivated by the work of Shafer [10]. This increase in dimension inevitably leads to a more complicated computation.

A similar basic idea has been previously studied [4]. However their approach was essentially a generalization of the c-table of Gragg [5]. Consequently the construction of the polynomial coefficients of quadratic approximation require the solution of determinants of order $(\ell+m+n+3)$.

In this chapter, the polynomial coefficients $P(\ell,m,n;x)$ are expressed by determinants of order $(\ell+m+2)$. These determinants are computed recursively by a general algorithm which is based on Brezinski's algorithm [2],[3],[8].

The concept of interpolation by a quadratic approximation is introduced. The same general algorithm can be used to calculate an interpolatory quadratic approximation. This leads naturally to extrapolation by quadratic approximation and hence to new methods of accelerating the convergence of slowly convergent sequences using either the basic quadratic approximation (essentially a generalization of the epsilon algorithm based on the Pade approximation) or the interpolatory quadratic approximation (a generalization of rational extrapolation based on a rational interpolating function).

There are several aspects of this work that are still being investigated. The approach to this problem was considered with a view to subsequent extensions to higher dimensions and this appears to be relatively straightforward with this algorithm.

However, other properties of approximations of this type appear to be less clearcut. For example in applications [6],[11] it is implicitly assumed that the (n,n,n) approximant is the best approximation from the variety of choices for quadratic approximation of order 3n + 2. However, numerical experiments have shown that this is not always true (compare example 2).

It may happen that some of the quadratic approximants $(\ell,m,n;x)$ are equal or do not exist. In these singular cases the algorithm breaks down. The extension of the treatment of the singular case in rational approximation [8][9] is still being studied.

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CHAPTER 7.

SOME PROPERTIES OF THE QUADRATIC APPROXIMATION AND COMPARISON WITH OTHER NON-LINEAR TRANSFORMATIONS

7.1 INTRODUCTION

Since quadratic approximation is an analogy of Pade approximation, they should have similar properties. The quadratic approximation is shown to have a similar weak linearity property.

This approximation is used to accelerate the convergence of sequences and series. These include both linearly and logarithmically convergent series, monotone and alternating series. Compared with other accelerators such as the u transform, the ε-algorithm and the θ algorithm [5], the results show that generally it gives better results than the ε, θ family of algorithms but it is not as good as the u transform.

7.2 THE PROPERTIES

The following properties of the Pade approximation extend to the quadratic approximation. Some of these have been noted by Gammel [2].

a) The equations determining the coefficients in the polynomials $\alpha(\ell,m,n;x)$, $\beta(\ell,m,n;x)$ and $\gamma(\ell,m,n;x)$ are linear. The power series expansion of f(x) is known; therefore the power series expansion of $f^2(x)$ is known, so the coefficients appear in (6.2.1) linearly.

b) The (n,n,n;x) quadratic approximant is invariant under homographic transformations $x = Ay/(1+By)$ [2]. These are used to expand the region of convergence in physics applications.

c) The quadratic approximants (n,m,n;x) to a unitary f(x) (one which satisfies $f(x)f^*(x) = 1$ for x real) are unitary [2].

d) The non-linear quadratic transformation of f(x) satisfies a weak linearity property. For convenience, the quadratic approximation of $f(x) = \sum_{i=0}^{\infty} C_i x^i$ can be considered as a quadratic transformation Q of f(x). Then it can be written in operator form

$$Q[f(x)] = \frac{-\beta \pm \sqrt{\beta^2 - 4\alpha\gamma}}{2\alpha}$$

If Q were linear, we would have

(i) $Q[Kf(x)] = KQ[f(x)]$

and (ii) $Q[f(x) + h(x)] = Q[f(x)] + Q[h(x)]$

where K is a constant and h(x) is a second function. Although (i) can be shown to be true, (ii) is not generally true. However Q satisfies the weaker rule:

$$Q[f(x) + K] = Q[f(x)] + K \qquad \text{for } \ell \leqslant m \leqslant n.$$

This property is an analogue of the non-linearity of the Shanks transform [4] which computes the Pade table (m,n) where $n \geqslant m$.

The proof of (i) and (ii) proceed as follows:

Proof:

(i) $Kf(x) = K\sum_{i=0}^{\infty} C_i x^i = KC_0 + KC_1 x + \ldots$

If the square of $\sum_{i=0}^{\infty} C_i x^i$ is $\sum_{i=0}^{\infty} A_i x^i$, then

$(K\sum_{i=0}^{\infty} C_i x^i)^2 = K^2 \sum_{i=0}^{\infty} A_i x^i = K^2 A_0 + K^2 A_1 x + \ldots.$

Let the polynomial coefficients of the quadratic approximation of $Kf(x)$ be $P'(\ell,m,n;x)$ where $P' = \alpha',\beta'$ and γ', then by (6.2.3),

$$\alpha'(\ell,m,n;x) = \frac{\begin{vmatrix} 0 & \ldots & 0 & x^{\ell} & \ldots & 1 \\ KC_{n-m+1} & \ldots & KC_{n+1} & K^2A_{n-\ell+1} & \ldots & K^2A_{n+1} \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ KC_{\ell+n+1} & \ldots & KC_{\ell+m+n+1} & K^2A_{m+n+1} & \ldots & K^2A_{\ell+m+n+1} \end{vmatrix}}{D} \qquad (7.2.1)$$

where D is the minor obtained by eliminating the first row and the last column of the numerator.

Multiply $\alpha'(\ell,m,n;x)$ and the first row of the numerator on the right hand side of (7.2.1) by k^2 and factorize the common factors K and K^2 from the columns. Then

$$K^2\alpha'(\ell,m,n;x) = \frac{K^{m+1}(K^2)^{\ell+1}}{K^{m+1}(K^2)^{\ell}}\,\alpha(\ell,m.n;x)$$

and $\qquad \alpha'(\ell,m,n;x) = \alpha(\ell,m,n;x)$

Now, replace the first row of the numerator in (7.2.1) by $(x^m \ldots 1, 0 \ldots 0)$ and multiply by K. Then

$$K\beta'(\ell,m,n;x) = \frac{K^{m+1}(K^2)^{\ell+1}}{K^{m+1}(K^2)^{\ell}}\,\beta(\ell,m,n;x)$$

and $\qquad \beta'(\ell,m,n;x) = K\beta(\ell,m,n;x)$

Again, replace the first row of the numerator in (7.2.1) by $-(Kx^m \sum_{i=0}^{n-m} C_i x^i \;\ldots\ldots\; K\sum_{i=0}^{n} C_i x^i,\; K^2 x^\ell \sum_{i=0}^{n-\ell} A_i x^i \;\ldots\; K^2 \sum_{i=0}^{n} A_i x^i)$.

Then $$\gamma'(\ell,m,n;x) = K^2\gamma(\ell,m,n;x).$$

So $$Q[Kf(x)] = \frac{-\beta' \pm \sqrt{\beta'^2 - 4\alpha'\gamma'}}{2\alpha'}$$

$$= K\left(\frac{-\beta \pm \sqrt{\beta^2 - 4\alpha\gamma}}{2\alpha}\right)$$

$$= KQ[f(x)]$$

(ii) $$f(x) + K = \sum_{i=0}^{\infty} C_i x^i + K$$

$$= (C_0 + K) + C_1 x + \ldots.$$

and $$(f(x) + k)^2 = \sum_{i=0}^{\infty} A_i x^i + 2K\sum_{i=0}^{\infty} C_i x^i + K^2$$

$$= (A_0 + 2KC_0 + K^2) + (A_1 + 2KC_1)x + \ldots$$

As before, let the polynomial coefficients of quadratic approximation of $f(x) + K$ be $P'(\ell,m,n;x)$ where $P' = \alpha', \beta'$ and γ'. Then

$$\alpha'(\ell,m,n;x) = \frac{\begin{vmatrix} 0 & \ldots & 0 & x^\ell & \ldots\ldots\ldots & 1 \\ C_{n-m+1} & \ldots & C_{n+1} & (A_{n-\ell+1} + 2KC_{n-\ell+1}) & \ldots & (A_{n+1} + 2KC_{n+1}) \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ C_{\ell+n+1} & \ldots & C_{\ell+m+n+1} & (A_{m+n+1} + 2KC_{m+n+1}) & \ldots & (A_{\ell+m+n+1} + 2KC_{\ell+m+n+1}) \end{vmatrix}}{D} \qquad (7.2.2)$$

Since for $\ell \leqslant m \leqslant n$, the ith column, where $i = m+1, \ldots,$ $m+\ell+2$, is the sum of itself and the multiple 2K of a corresponding column (i.e. the indices i of C_i and A_i are the same) in the first m columns.

$$\therefore \alpha'(\ell,m,n;x) = \alpha(\ell,m,n;x)$$

Replace the first row of the numerator in (7.2.2) by $(x^m \ldots 1, 0 \ldots 0)$ multiply the ith column, for $i = 1,\ldots,m$, by $(-2K)$ and add to a corresponding column in the last $(\ell+2)$ columns. Then

$$\beta'(\ell,m,n;x) = \frac{\begin{vmatrix} x^m, & \ldots & 1 & -2Kx^\ell & \ldots & -2K \\ C_{n-m+1} & \ldots & C_{n+1} & A_{n-\ell+1} & \ldots & A_{n+1} \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ C_{\ell+n+1} & \ldots & C_{\ell+m+n+1} & A_{m+n+1} & \ldots & A_{\ell+m+n+1} \end{vmatrix}}{D}$$

$$= \beta(\ell,m,n;x) - 2K\alpha(\ell,m,n;x)$$

Now, replace the first row of the numerator in (7.2.2) by $-(x^m(\sum_{i=0}^{n-m} C_i x^i + k), \ldots, \sum_{i=0}^{n} C_i x^i + k,\ x^\ell(\sum_{i=0}^{n-\ell} A_i x^i + 2K\sum_{i=0}^{n-\ell} C_i x^i + k^2), \ldots, \sum_{i=0}^{n} A_i x^i + 2K\sum_{i=0}^{n} C_i x^i + k^2)$. Using the same operations as above, then decompose for numerator to give

$$\gamma'(\ell,m,n;x) = \gamma(\ell,m,n;x) - K\beta(\ell,m,n\ x) + K^2\alpha(\ell,m,n;x)$$

Hence $$Q[f(x) + K] = \frac{-\beta' \pm \sqrt{\beta'^2 - 4\alpha'\gamma'}}{2\alpha'},$$

and since
$$\alpha'(\ell,m,n;x) = \alpha(\ell,m,n;x)$$
$$\beta'(\ell,m,n;x) = \beta(\ell,m,n;x) - 2K\alpha(\ell,m,n;x)$$
$$\gamma'(\ell,m,n;x) = \gamma(\ell,m,n;x) - K\beta(\ell,m,n;x) + K^2\alpha(\ell,m,n;x)$$

we obtain $Q[f(x) + K] = Q[f(x)] + K$ for $\ell \leqslant m \leqslant n$.

7.3 NUMERICAL TEST RESULTS

Several methods for accelerating the convergence of sequences and series have been tested and compared on a wide range of test problems by Smith and Ford [5]. This study included both linear and nonlinear methods. The linear methods were the generalized Euler transformation λ, the extended Salzer summation and Toeplitz arrays with entries obtained from Chebyshev or Legendre polynomials. The nonlinear methods, all generalizations of Aitken's Δ^2 method, included the ε-algorithm [4], [6] and its relatives ρ and θ and the Levin transforms t, u, v [3]. The test problems include both linearly and logarithmically convergent series, monotone and alternating series. Their results showed that Levin's u transform is the best, closely followed by the v transform. Among the $\varepsilon, \rho, \theta$ family, the only general purpose method is the θ algorithm and it turns out to be generally better than ε on problems to which they both can be applied. (The comparison of results from the linear and other methods can be obtained from [5]). Since the quadratic transform is the analogy of the ε-algorithm, it should belong to the same family.

In this section, the quadratic transform is tested on the same range of test problems and compared with the ε and θ transforms from the same family, and the u transform. The numerical results show that the behaviour of quadratic transform is similar to the $\varepsilon, \rho, \theta$ transform. The results are not as good as u transform but better than the ε and θ transforms on problems to which they can be applied. The results for the test problems by using the u transform, the θ and ε-algorithms, were obtained from [5]. The algorithms were computed in standard Fortran double precision on an IBM 360 system and compared with the results of the quadratic transform which was computed in standard Fortran double precision on a Prime computer up to 14 digits and on Burroughs 6700 for more than 14 significant digits.

a) Alternating series.

This group of test problems consists of series of the form $\sum_{n=1}^{\infty}(-1)^{n+1}a_n$ where a_n is defined in table 7.3.1.

Table 7.3.1.

No	a_n	S
1	$1/n$	0.693147180559945...
2	$1/(2n-1)$	0.785398163397448...
3	$1/\sqrt{n}$	0.60489864342162...
4	$\binom{-\frac{1}{2}}{n-1}\frac{(-1)^{n+1}}{n}$	0.828427124746190...
5	$\binom{-\frac{1}{2}}{n-1}^2$	0.834626841674073...

In the following figure (figure 7.3.1) the graphs show significant digits of the answer as a function of the number of terms of the series actually used. The graphs of the u,θ,ε transforms are obtained from [5] while the graph of the quadratic is obtained from selecting the best transform from among those using the same number of terms of the original series. The best transform (ℓ,m,n) on problem (1) - (3) and (5) is selected from $(k+1)(k+2)/2$ terms where $k = \ell+m+n$. But the selection on problem (4) is only from $(0,m,n)$ since in the computation of $(1,0,n)$ a singularity appears and the algorithm breaks down.

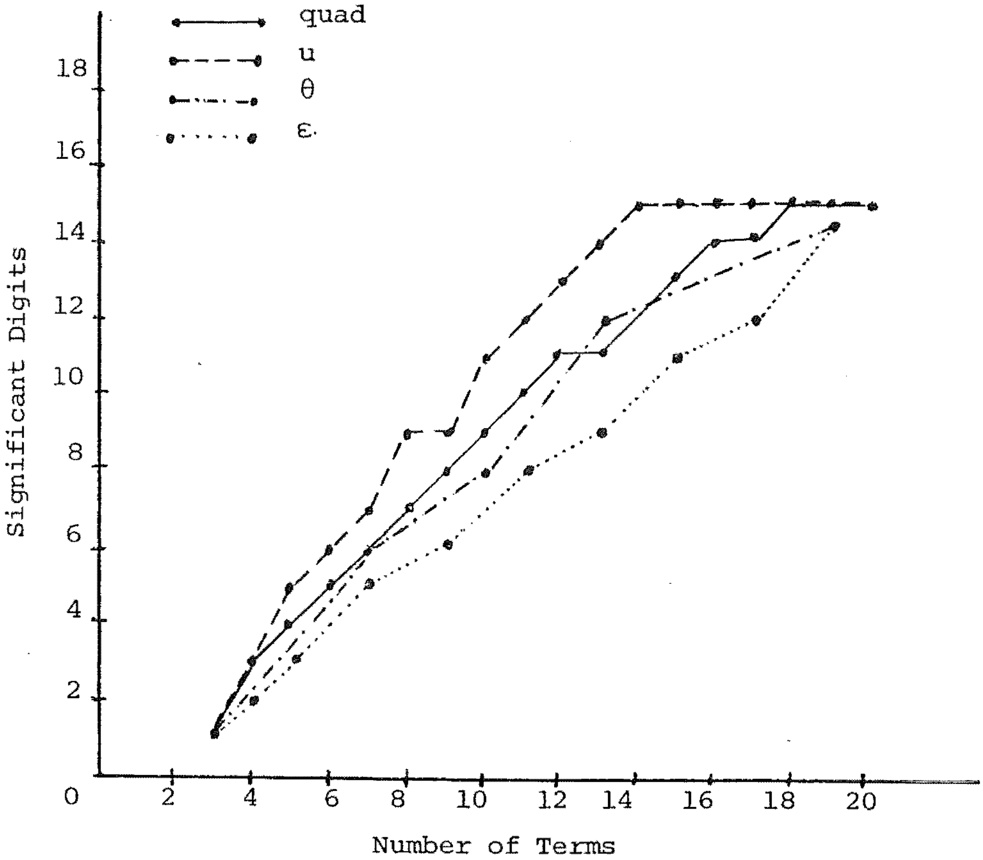

Figure 7.3.1.

Performance of nonlinear accelerators on alternating series, averaged over problems (1) - (5). *Significant digits of correct answer are shown as a function of number of terms of the series used.*

It can be seen from the graphs that the quadratic transform is quite successful in accelerating the convergence of an alternating series. These results were computed on a Prime computer which has a similar arithmetic structure to the IBM 360 system.

b) Logarithmic convergence.

The logarithmically convergent test problems are shown in Table 7.3.2.

Table 7.3.2

No.	a_n	S
6	$1/n^2$	1.644934066848226
7	$\frac{1+n^2+n^4}{n^2(1+n^4)}$	2.223411647...
8	$\frac{2n-1}{n(n+1)(n+2)}$	0.75
9	$\sin\frac{1}{n}\,\ln\cos\frac{1}{\sqrt{n}}$	-0.852090754...
10	$(n+e^{1/n})^{-\sqrt{2}}$	1.71379673554030...

The quadratic transform failed on all of them. That is it did not extract more than two significant digits of the correct answer from 20 terms of the series. The ε-algorithm also fails on all these problems [5].

c) Linear monotone convergence.

Three monotone series $\sum_{n=1}^{\infty} a_n$ that converge linearly are considered in Table 7.3.3.

Table 7.3.3.

No.	a_n	S
11	$n(0.8)^{n-1}$	25
12	$(0.4)^{n-1} + (0.8)^{n-1}$	20/3
13	$(0.8)^n/n$	$\ln 5$

The u,ε and λ algorithms all give exact results on problem (11). The quadratic algorithm gives 10 significant digits by using 4 terms. For problem (12), the ε-algorithm is exact. The quadratic algorithm gives 9 significant digits by using 5 terms and 10 significant digits by using 7 terms.

The numerical results for problem (13) are shown in Table 7.3.4.

Again, the results show that the quadratic algorithm is in-between the u and ε-algorithms.

Table 7.3.4.

Number of terms	Significant digits			
	u	quad.	ε	θ
11	6	6	4	
12	6	7		
13	7	7	5	6
14	7	7		
15	8	7	7	
16	9	8		6
17	9	8	7	
18	10	8		
19	10	9	8	6
20	11	10		

7.4 CONCLUSION

As noted in [5], it is difficult to provide firm proof for many intuitive conclusions about sequence accelerators, especially nonlinear ones. If $\sum_{i=0}^{\infty} c_i x^i$ is the series expansion of a quadratic function with coefficients at most ℓ, m, n respectively, then it follows that the quadratic approximation algorithm sums the series exactly at least when it reaches the $(\ell, m, n; x)$ approximant.

The numerical results show that generally the quadratic algorithm is as good as the ε-algorithm but not as good as Levin's u transform. With the development of this algorithm the determination of these situations where the quadratic transformation is advantageous remains to be investigated. Some further questions include:

1. The Levin u,v,t transforms are in some sense, a generalization of the well-known transformation due to Shanks , which turns out to be the ε-algorithm. The quadratic transform is the higher dimensional analogue of the ε-algorithm. It may be possible to generalize the quadratic transform in a way similar to u,v,t transforms.

2. Among the $(k+1)(k+2)/2$ possibilities (where $k = \ell+m+n$) for the quadratic approximation of a given order, which one gives the best result? Can this be predicted from the given information such as the behaviour of the series or sequence?

3. How can the best result be automatically selected? At least one attempt at this problem has been made [1].

4. The quadratic transform can be extended to cubic and quartic transforms. As the dimension is increased, the algorithm becomes much more complicated. However, the basic algorithm from this study should be valuable for future investigations.

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